

An introduction to programming in R

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Contents

1	Introduction	3
1.1	Getting and installing R	4
1.2	Getting and installing Rstudio	4
1.3	First interactive calculations	4
2	Scripts and data files	8
2.1	More R basics: functions and their documentation	12
2.2	Statistics in R	14
3	Common R Objects: Vectors, Matrices, and Data Frames	15
3.1	Vectors	15
3.1.1	Functions for creating vectors	15
3.1.2	Vector addressing	16
3.2	Matrices	18
3.2.1	Creating matrices	18
3.2.2	<code>cbind</code> and <code>rbind</code>	19
3.2.3	Matrix addressing	20
3.3	Operations with Matrices and Vectors	21
3.3.1	Eigenvalues and eigenvectors	22
3.3.2	Eigenvector scalings	25
3.3.3	Eigenvalue sensitivities and elasticities	25
3.4	<code>matrix</code> or <code>Matrix</code> ? Classes in R	26
3.5	Data Frames (and more R tricks)	28

¹Some of these notes are largely copied – verbatim at times – from 2015 and earlier versions of *An introduction to R for theoretical ecology* and associated online materials by my Ph.D. advisor Stephen P. Ellner and his co-author John Guckenheimer. That document can be found online at <https://github.com/ellner/DMB-supplements/blob/master/Lab%20Manual/DynamicModelsLabsInR%3D2019.pdf>, and is based in part on course materials by Ellner’s former TAs Colleen Webb, Jonathan Rowell and Daniel Fink at Cornell, Lou Gross (University of Tennessee) and Paul Fackler (NC State University), and on the book *Getting Started with Matlab* by Rudra Pratap (Oxford University Press). Here I also draw heavily from the documentation supplied with **R**, and from [Ecological Models and Data in R](#) © Benjamin M. Bolker.

3.5.1	Data frame addressing	28
3.5.2	More on vector, matrix and data frame addressing	29
4	Iteration (“Looping”)	31
4.1	For-loops	31
4.2	While-loops	34
4.2.1	Logical operators	35
4.3	Iteration alternatives in R: flavors of <code>apply()</code>	37
5	Branching: using <code>if</code> and <code>else</code>	38
5.1	Nested <code>if</code> statements	38
5.2	Functions <code>ifelse()</code> and <code>switch()</code>	39
6	Writing your own functions	41
7	Solving differential equations	43
7.1	Always use <code>lsoda!</code> Except when you shouldn’t...	44
7.2	The logs trick	45
7.3	Additional arguments in <code>lsoda</code>	46
8	Optimization and fitting models to data	47
8.1	What to optimize?	49
8.2	Controlling the optimization	50
8.3	How to optimize	51
9	Document Creation in Rstudio	52
9.1	R Markdown	52
9.2	knitr/Sweave Documents (L ^A T _E X with embedded R code & output)	52
	References	53

1 Introduction

The notes are a modification of materials provided by Stephen P. Ellner, which themselves include contributions from former TAs Colleen Webb, Jonathan Rowell and Daniel Fink at Cornell, Professors Lou Gross (University of Tennessee) and Paul Fackler (NC State University), and the book *Getting Started with Matlab* by Rudra Pratap (Oxford University Press). They also draw on the documentation supplied with R. These notes also overlap with the notes on R that accompany the textbook *Dynamic Models in Biology* by Steve Ellner and John Guckenheimer (Princeton University Press 2006). You can freely download that computer lab manual (versions for R and for Matlab) and the various R scripts and data files mentioned below at:

<https://github.com/ellner/DMB-supplements/>

These notes are written under the assumption that you have a computer (running R) in front of you. It is important to work through examples yourselves - **i.e. type them into R and see what happens on your screen** - to get the feel and experience of working in R. Exercises or examples in the middle of a section (here or in the text) should be done immediately when you get to them, making sure you have them right before moving on. Additional exercises may be given at the end of some sections.

These notes also refer to the text *Ecological Models and Data in R* by Benjamin Bolker © 2008, and should follow either the published text or the draft book chapters available as PDFs at <http://ms.mcmaster.ca/~bolker/emdbook/>

This document is a constant work-in-progress, so please reach out and contact me (Paul Hurtado) if you find any errors or have suggestions for improvements.

What is R? R is an object-oriented scripting language that combines

- the S programming language developed by John Chambers (Chambers and Hastie 1988, Chambers 1998).
- a user interface with a few basic menus and extensive help facilities.
- an enormous set of functions for classical and modern statistical data analysis and modeling.
- graphics functions for visualizing data and model output.

R is an open-source project (R Core Development Team 2017) available free via the Web. Originally a research project in statistical computing (Ihaka and Gentleman 1996) it is now managed by a team that includes many well-regarded statisticians, and is widely used by statistical researchers and a growing number of theoretical biologists. The commercial implementation of the S language (called S-plus) offers a “point and click” interface that R lacks. However for our purposes this is outweighed by the fact that S-plus still lacks some essential tools for simulating dynamic models. The standard installation of R includes extensive documentation, including an introductory manual and a comprehensive reference manual. At this writing, R mostly follows version 3 of the S language, but some packages are starting to use version 4 features. *These notes refer only to version 3 of S.* We also limit ourselves to graphics functions in the base graphics package; much more is available in packages such as **ggplot2**, **lattice** and **grid**.

What is Rstudio? Rstudio (www.rstudio.com) is a free, advanced user interface for R. Syntax highlighting, autocompleting, document creation, and various other functionalities make Rstudio a very helpful user interface that can speed up the learning process for new R users. I strongly recommend that all of your work in R be done using Rstudio.

1.1 Getting and installing R

The main sources for R are CRAN (<http://www.cran.r-project.org>) and its mirrors. You can get the source code, but most users will prefer a precompiled version. To get one from CRAN, click on the link for your OS, continue to the folder corresponding to your OS version, and find the appropriate download file for your computer.

For Windows or OS X, R is installed by launching the downloaded file and following the on-screen instructions. At the end you'll have an R icon on your desktop that can be used to launch the program. Installing versions for LINUX or UNIX is more complicated and idiosyncratic (which will not bother the corresponding users), but many LINUX distributions include a fairly up-to-date version of R.

During installation, it's common to select a "custom" install and change the default setting from SDI (single window with multiple subwindows) to MDI (multiple windows). This allow R's command and graphics windows to move independently on the desktop, and you can also change this in R by modifying the *GUI preferences* in the drop-down menu.

This document was written on a Windows PC and sometimes refers to Windows-specific aspects of R; please let me know about any OS-related issues so I can correct them.

1.2 Getting and installing Rstudio

Rstudio can be downloaded for free from <https://www.rstudio.com/>, and should be installed after R. If you are interested in using Rstudio to create professional looking documents with nicely formatted equations and R output, you should also install a \LaTeX distribution (e.g., MikTeX on Windows PCs) and then install Rstudio. We'll talk more about document creation in section 9. See the Resources page on the Rstudio website for additional helpful cheatsheets, examples, and tutorials.

1.3 First interactive calculations

When R is launched it opens the *console* window. This has a few basic menus at the top, whose names and content are OS-dependent; check them out on your own. The console is where you enter commands for R to execute *interactively*, meaning that the command is executed and the result is displayed as soon as you hit the Enter key. For example, at the command prompt `>`, type in `2+2` and hit Enter; you will see

```
> 2+2
[1] 4
```

To do anything complicated, the results from calculations have to be stored in variables. For example, type `a=2+2; a` at the prompt and you see

```
> a=2+2; a
[1] 4
```

The variable `a` has been created, and assigned the value 4. The semicolon allows two or more commands to be typed on a single line; the second of these (`a` by itself) tells R to print out the value of `a`. By default, a variable created this way is a vector (an ordered list of numbers); in this case `a` is a vector length 1, which acts just like a number.

There are some rules for giving names to variables:

- Variable names in R must begin with a letter, and followed by alphanumeric characters. Long names can be broken up using a period, as in `very.long.variable.number.3`.
- **Do not** use the underscore character ('_') or blank space as a separator in variable names (R will probably give you an error message if you do).
- R is case sensitive: `Abc` and `abc` are **not** the same variable.

Calculations are done with variables as if they were numbers. R uses `+`, `-`, `*`, `/`, and `^` for addition, subtraction, multiplication, division and exponentiation, respectively. For example enter

```
> x=5; y=2; z1=x*y; z2=x/y; z3=x^y; z2; z3
```

and you should see

```
[1] 2.5
[1] 25
```

Even though the values for `x`, `y` were not displayed, R “remembers” that values have been assigned to them. Type `> x; y` to display the values.

The `↑` key recalls previous commands to the prompt, so they can be corrected or modified. For example, you can bring back the next-to-last command and edit it to

```
> x=5 y=2 z1=x*y z2=x/y z3=x^y z2 z3
```

so that commands are not separated by a semicolon. Then press Enter, and you will get an error message.

You can do several operations in one calculation, such as

```
> A=3; C=(A+2*sqrt(A))/(A+5*sqrt(A)); C
[1] 0.5543706
```

The parentheses are specifying the order of operations. The command

```
> C=A+2*sqrt(A)/A+5*sqrt(A)
```

gets a different result – the same as

```
> C=A + 2*(sqrt(A)/A) + 5*sqrt(A).
```

The default order of operations is: (1) Exponentiation, (2) multiplication and division, (3) addition and subtraction.

```
> b = 12-4/2^3           gives    12 - 4/8 = 12 - 0.5 = 11.5
> b = (12-4)/2^3       gives    8/8 = 1
> b = -1^2             gives    -(1^2) = -1
> b = (-1)^2           gives    1
```

It’s generally best to *use parentheses to specify exactly what you want*, such as

```
> b = 12 - 4/(2^3) .
```

R also has many **built-in mathematical functions** that operate on variables (see Table 1). You can get help on any R function by entering

```
?functionname
```

in the console window (e.g., try `?sin`). You should also explore the items available on the Help menu, which include the manuals, FAQs, and a Search facility (‘Apropos’ on the menu) that is useful if you sort of maybe remember part of the the name of what it is you need help on.

<code>abs(x)</code>	absolute value
<code>cos(x), sin(x), tan(x)</code>	cosine, sine, tangent of angle x in radians
<code>exp(x)</code>	exponential function
<code>log(x)</code>	natural (base-e) logarithm
<code>log10(x)</code>	common (base-10) logarithm
<code>sqrt(x)</code>	square root

Table 1: Some of the built-in mathematical functions in **R**. Use the Help system to get a more complete list: `?Arithmetic` for simple functions, `?log` for logarithmic, `?sin` for trigonometric, and `?Special` for special functions.

Exercise 1.1: Have R compute the values of

1. $\frac{2^7}{2^7-1}$ and compare it with $\frac{1}{1-2^{-7}}$.
2. $\sin(0.25)$, $\cos^2(0.5)$ [Note that typing `cos^2(0.5)` won't work!]
3. $\frac{2^7}{2^7-1} + 4\sin(0.25)$, using cut-and-paste to assemble parts of your past commands.

Exercise 1.2: Do an `Apropos` on `sin` via the Help menu, to see what it does. Next, enter the command `help.search("sin")` and see what that does (answer: `help.search` finds *all* Help pages that include 'sin' anywhere in their title or text, most having nothing to do with trig functions. `Apropos` just finds functions that have 'sin' somewhere in their name).

Exercise 1.3: Work through the *Sample Session* at the end of Bolker, Chapter 1. Use the help system (or your neighbor) to do a linear regression of the *frog-tadpole* data. I have included those simulated data below so that you can copy/paste them into R. Try entering `help.search("fitting linear models")` or `?lm` in the R console.)

```
frogs = c(1.1, 1.3, 1.7, 1.8, 1.9, 2.1, 2.3, 2.4, 2.5, 2.8, 3.1, 3.3, 3.6, 3.7, 3.9,
          4.1, 4.5, 4.8, 5.1, 5.3)
tadpoles = c(2.036982, 2.876231, 3.062528, 3.707180, 3.955385, 4.786983, 4.909395,
             4.743633, 5.458514, 5.488370, 6.463224, 6.202578, 7.913878, 6.666590,
             7.681658, 8.103331, 8.575123, 9.629233, 9.791165, 9.574846)
```

Reading² Assignment: Bolker, Chapter 1

- Read pages 1-4 (1-4)
- Skim pages 4-17 (4-20)
- Read 17-22 (20-26).

²As a convention, book chapters and page numbers will be given for the printed version of the text, followed by the corresponding chapters and page numbers for online version in parentheses.

2 Scripts and data files

Scripts and data files mentioned below refer to supplementary materials for the textbook *Dynamic Models in Biology* (<https://github.com/ellner/DMB-supplements/>). These files can be downloaded using this link: <https://github.com/ellner/DMB-supplements/tree/master/LabRFiles>.

Modeling and complicated data analyses are more easily done using *scripts*: a series of commands stored in a text file. The Windows and OS X versions of R include a basic script editor (accessed via the **file** menu on the console), but you can also use an external text editor.

Most scripts for working with models or data follow a simple pattern:

1. “Setup” statements.
2. Load some data from a file (or keyboard input).
3. Carry out the desired calculations.
4. Output of numerical results and associated graphics, perhaps saving them to files.

For example, a script file might

1. Load some packages, or run another script file that creates some functions (more on functions later).
2. Read in from a text file the parameter values for a predator-prey model, and the numbers of predators and prey at time $t = 0$.
3. Calculate the population sizes at times $t = 1, 2, 3, \dots, T$.
4. Graph the results and save the graph as a PDF file for including in your term project.

Here is a simple script you can create by opening up Rstudio and creating a new R script by selecting **File > New File > R Script** (or you can use the shortcut **Ctrl-Shift-N**) and entering the following text into the empty script window (top panel, above the console).

```
# This simple script plots a histogram for a Normally distributed random sample
# FYI: Lines that start with a '#' are comments, and are not parsed as R code

# Simulate the random sample of size 250 with mean = 12, standard deviation = 1
mysample = rnorm(250, mean=12, sd=1)

# Plot the histogram. See R documentation for 'hist' and 'seq' for details
hist(mysample,breaks=seq(0,20,by=0.5))
```

Use the icons at the top of the script window in R Studio to run the script. You can also run the script using **Ctrl-shift-enter** or run it line-by-line using **Ctrl-r** or **Ctrl-enter** to run the current line based on the cursor location.

For another example, download and open the file **Session1.1.R** has the commands from the interactive regression analysis. **Important:** before working with an example file, create a personal copy in some location on your own computer. We will refer to this location as your *temp folder*. If working on a computer in a computer lab, at the end of your lab session you may want to save files onto flash drive, email them to yourself, or upload them to your preferred storage in the cloud.

Open *your copy* of **Session1.1.R**, using **File/Open Script** from the console menu. On the **Edit** menu of the script editor, select **Run All**. This equivalent to copying the whole script and pasting it into the console window, so the commands are all executed and a graph is displayed with the results. The **source** function runs an entire script file without copying it to the console, e.g.

```
> source("c:/temp/Session1.1.R")
```

Source'ing can also be done in point-and-click fashion via **File/Source R code** on the console window.

Another important time saver is loading data from a text file. Get copies of **Session1.2.R** and **ChlorellaStart.txt** to see an example of how this can be done. In **ChlorellaStart.txt**, time and algal density are entered as two columns of a data matrix. Then instead of typing these in by hand, the command

```
X=read.table("c:/temp/ChlorellaStart.txt")
```

reads the data file and puts the data values into the variable **X**. Note that the path to the data file has to be specified; you need to edit the script so that it uses the correct path to your data file. There are two ways to specify paths: a single forward slash (as in the **source** command just above), or a double backslash as in the **read.table** command. R understands both of these, but a single backslash won't work. In the console window, do

```
> X
```

to see that **X** has been loaded into R as a data matrix with two columns. **V1** and **V2** are “default” variable names that R has assigned to the two columns.

The variables are then extracted from **X** with the commands

```
tvals=X[,1]; cvals=X[,2];
```

These are shorthand for “tvals = everything in column 1 of **X**”, and “cvals = everything in column 2 of **X**” (you'll learn about working with matrices later). The rest is the same as before, with some additions that specify axis labels and a title.

Exercise 2.1 Make a copy of **Session1.2.R** under a new name, and modify the copy so that it plots algal density versus time and does linear regression of algal density on time, and plots the data appropriately. As in **Session1.2.R**, use only the first 5 data points for the linear regression. You should end up with a graph sort of like Figure 1.

Exercise 2.2 Run **Session1.2.R**, then enter the command **plot(fit)** in the console. R will tell you that it is “Waiting to confirm page change” – help it out by clicking on the plot to do a page change. Next, figure out what just happened by entering **?plot.lm** to bring up the Help page for the function **plot.lm** that carries out a **plot** command for an object produced by **lm**. [This is one example of how R uses the fact that data analyses are stored as model objects. **fit** “knows” what kind of object it is and **plot(fit)** invokes a function that produces plots suitable for an object produced by **lm**.] **Answer:** R produced a series of diagnostic plots exploring whether or not the fitted linear model is a suitable fit to the data. In each of the plots, extreme points (the most likely candidates for “outliers”) have been identified according to their sequence in the data set.

Finally, we want to see how well a discrete logistic model fits the data. To see how that can be done, look at **Session1.3.R**. The first sections are familiar: reading in the data and finding the parameter values. Then comes something new: a “for-loop” to solve the model by stepping forward one day at a time, starting from our estimated value at $t = 0$. We'll learn about this later – for now, just take it for granted:

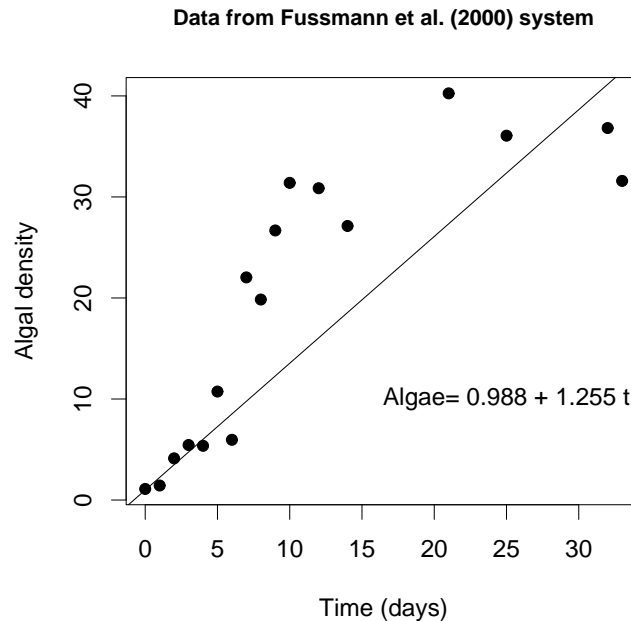


Figure 1: Graphical summary of regression analysis without log transformation.

```
xvals=numeric(34); xvals[1]=x0;
for(j in 2:34) {xvals[j]=R*xvals[j-1]*(1-b*xvals[j-1])}
```

The part to notice now is how to put the data and model solutions onto the same plot:

```
plot(tvals,cvals,type="p",pch=16,cex=1.5, col="green",xlab="Time (days)",ylab="Algal density");
points(0:33,xvals,type="o",pch=16,cex=1,col="black",lwd=2);
```

The `plot` command is familiar with one new wrinkle: the “col” variable sets the plotting color. The `points` function is just like `plot` except that it adds new points (or lines) to the most recent plot, rather than making a new plot.

Exercise 2.3 The axes in plots are scaled automatically, but sometimes you want to control them yourself, for example you may want several graphs with exactly the same axes limits. You can control scaling using the `xlim` and `ylim` arguments in `plot`: the general syntax is

```
plot(x,y,xlim=c(x1,x2), ylim=c(y1,y2))
```

For example,

```
plot(x,y,type="l",xlab="x",ylab="y",xlim=c(1,5), ylim=c(.2,1))
```

will draw a graph with the x-axis going from 1 to 5, the y-axis from 0.2 to 1.0. The file **Chlorella-Growth.txt** has data on the maximum algal growth rate r_{max} as a function of light intensity L . Write a script that loads these data into R, and creates a plot of growth rate versus light intensity with the x axis running from 0 to 120, and the y axis running from 1 to 4. Save this script for use in the next exercise.

Exercise 2.4 Several separate graphs can be placed within a single figure by using the `par` function (short for “parameter”) to adjust the layout of the plot. For example the command

```
par(mfrow=c(m,n))
```

divides the plotting area into m rows and n columns. Then as a series of `plot` commands are used to draw graphs, successive graphs are placed along the top row from left to right, then along the next row, and so on. `mfcol=c(m,n)` has the same effect except that successive graphs are placed down the first

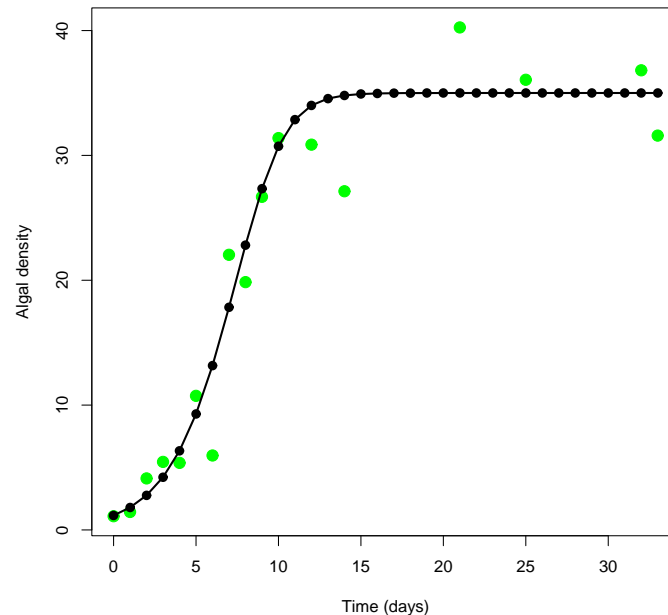


Figure 2: Discrete logistic model (black curve) fitted to experimental data on *Chlorella* growth from the Fussmann et al. (2000) experimental system (green points).

column, then down the second column, and so on. `par` can't be put inside of a `plot()` command – it has to be separate and it has to come before the plots are drawn.

Save a copy of your script from the last exercise under a new name, and modify it as follows. Use `mfc01=c(2,1)` to create graphs of (1) growth rate as a function of Light, and (2) $\log(\text{growth rate})$ as a function of $\log(\text{Light})$, within one figure. Do the same again, using `mfc01=c(1,2)`.

Exercise 2.5 Use `?par` to read about other plot control parameters that can be set using `par()`. Then draw a 2×2 set of plots, each showing the line $y = 5x + 3$ with x running from 3 to 8, but with 4 different line styles and 4 different line colors. (Note: if $x=3:8$, then $y=5*x+3$ will create the y values that you need).

Exercise 2.6 Modify one of your scripts so that at the very end it saves the plot to disk. In Windows, this can be done using `savePlot`; for other OS's, you can use `dev.print`. Use the Help system to find out about these functions (e.g., `?savePlot`). Note that the argument `filename` in `savePlot`, and the argument `file` in `dev.print`, can include the path to a folder, for example in Windows you can use `filename="c:/temp/MyFigure2"`.

Note: These are really exercises in using the Help system, with the bonus that you learn some things about `plot`. (Let's see, we know `plot` can graph data points...maybe it can also draw a line to connect the points, or just draw the line and leave out the points. That would be useful. So let's try `?plot` and see if it says anything about lines...Hey, it also says that **graphical parameters can be given as arguments to plot**, so maybe I can set line colors inside the plot command instead of using `par` all the time....). The Help system is *very* helpful once you get used to it (which takes a while), and acquire the habit of using it often.

2.1 More R basics: functions and their documentation

As seen above, R has a nice help system that can be queried in multiple ways. From the command line, these include:

```
> help.search("search string")
> ?function.name
> apropos("search string")
```

To best utilize the help pages for specific functions, let us take a closer look at what functions are and how they work.

At the command line, type the name of the function `read.csv`, no parentheses. You should get something like

```
> read.csv
function (file, header = TRUE, sep = ",", quote = "\"", dec = ".",
  fill = TRUE, comment.char = "", ...)
read.table(file = file, header = header, sep = sep, quote = quote,
  dec = dec, fill = fill, comment.char = comment.char, ...)
<environment: namespace:utils>
```

Typing the function name alone returns code for the function³. Typing `?read.csv` loads the help file, which gives a more useful overview of what arguments you give `read.csv`, and what values it returns.

Each function takes a set of arguments, which may or may not have a default value, and returns some object. In this case, `read.csv` is a function that reads in data from a comma separated file and stores it as a variable in R. In this case, `file` is the name of the file to open, `header` is a logical (true/false) variable indicating whether or not the first row is data or column names, and so on. Here `file` has no default file name, whereas `header=TRUE` means that if omitted, the function assumes the first row gives the column names.

See the help for `write.csv`. One could create a CSV file from the simulated frog-tadpole data from exercises above using the following command (use `file=""` to display to the console instead)

```
> write.csv(data.frame(frogs,tadpoles), file="frog-tadpole.csv", row.names=FALSE)
```

If you had a CSV file of data **without labeled columns** in the *working directory*⁴, you could load it into a variable `my.data` and display the contents to the screen by typing

```
> my.data = read.csv(file="frog-tadpole.csv");
> my.data
```

If the first row in the CSV file contained the first row of data instead of column labels, you would use

```
> my.data = read.csv(file="frog-tadpole.csv", header=F);
> my.data
```

³Compare this to typing `read.csv()` and `read.csv`

⁴First, type `getwd()` at the command line to see what your current “working directory” is. If you need to change it, use `setwd()`. Next, go to the course website and download the `frog-tadpole.csv` file to that directory. Edit the directory name in the example code accordingly.

In the first case, the default `header=T` told `read.csv` to take the first row as the column names. Variable names (and thus, column names) can't start with a number in R. If the column labels had been omitted from the file, they would have received column names like `X1.1` and `X2.036981755`. In the second case, if we treated the labels like data, the columns received the default labels `V1` and `V2`. We can change these by

```
> names(my.data)
> names(my.data) = c("frogs", "tadpoles");
> my.data
```

However, it's always preferable to open the files correctly. When in doubt, or if you run into problems, **loading the help documentation for the function in question should be your first step towards solving the problem.**

Exercise 2.7: The best way to get a feel for how functions work is to create your own. Here we'll create a function `square` that returns the square of it's argument, or if no argument is given the default value is a random integer from 0 and 10. This defines the function:

```
> square = function(x = round(runif(1,min=0,max=10)) ) {
>   return(x^2);
> }
```

What happens when you type the following?

```
> square(12)
> square()
> square
```

Exercise 2.8: Plot our data using `plot(my.data)`. Read the help for the `plot` command, and plot it with a new title and axis labels of your choosing.

2.2 Statistics in R

Some of the important functions and packages for statistical data analysis are summarized in Table 2. The book *Modern Applied Statistics with S* by Venables and Ripley gives a complete practical overview. For the basics Maindonald (2004) and Verzani (2002) are available free from CRAN (www.cran.r-project.org), and you can also find there a complete list of libraries and their contents (click on **Package sources**). There is also a large collection of R packages for the analysis of genomic data distributed at www.bioconductor.org. For the most part, we will not go too deeply into this side of R - at least until later in the course.

aov, anova	Analysis of variance or deviance
lm, glm	Linear and generalized linear models
gam, gamm	Generalized additive models and mixed models (in mgcv package)
nls	Fit nonlinear models by least-squares (in nls package)
lme, nlme	Linear and nonlinear mixed-effects models (in nlme package)
foreign	Read Data Stored by Minitab, S, SAS, SPSS, Stata, etc
sp	tools for spatial data
forecast, zoo	time series analysis
reshape2	Reshape data into different formats
plyr	More data manipulation tools
boot	Functions for bootstrap estimates of precision and significance
multiv	Multivariate analysis
survival	Survival analysis
tree	Tree-based regression
MASS, AER, car	Statistics textbook companion packages
nonparametric regression	Various functions in numerous libraries including stats (smoothing splines, loess, kernel), mgcv , fields , KernSmooth , logspline , sm
Rcmdr	R Commander: Point-and-click GUI for basic statistics and model fitting, can import data from SPSS, Minitab or STATA data files

Table 2: A small selection of the functions and add-on packages in **R** for statistical modeling and data analysis. There are **many** more, but you will have to learn about them somewhere else. A number of free manuals are available at CRAN www.cran.r-project.org.

3 Common R Objects: Vectors, Matrices, and Data Frames

Understanding how to use vectors and matrices is fundamental to capitalizing on R's computational abilities and for doing scientific computing in general. That said, the data frame is also common to work with in R. In this next section, we get familiar with all three.

3.1 Vectors

Vectors and matrices (1- and 2-dimensional rectangular arrays of numbers) are pre-defined data types in R. We've already seen two ways to create vectors in R:

1. A command in the console window or a script file listing the values, such as

```
> initialsize=c(1,3,5,7,9,11).
```

2. Using `read.csv()`:

```
> my.data=read.csv("frog-tadpole.csv")
```

(**Remember:** this only works if the file that you're trying to read actually exists!)

A vector can then be used in calculations as if it were a number (more or less)

```
> finalsize=initialsize+1; newsize=sqrt(initialsize); finalsize; newsize;
[1] 2 4 6 8 10 12
[1] 1.000000 1.732051 2.236068 2.645751 3.000000 3.316625
```

Notice that the operations were applied to every entry in the vector. Similarly, commands like `initialsize-5`, `2*initialsize`, `initialsize/10` apply subtraction, multiplication, and division to each element of the vector. The same is true for

```
> initialsize^2;
[1] 1 9 25 49 81 121
```

In R the default is that operations and functions act on vectors in an *element by element* manner; anything else (e.g. matrix multiplication) is done using special notation (discussed below). Note: **this is the opposite of MATLAB**. In MATLAB, matrix operations are the default and element-by-element operations require special notation.

3.1.1 Functions for creating vectors

A set of regularly spaced values can be created with the `seq` function, whose syntax is

```
x=seq(from,to,by) or x=seq(from,to)
```

The first form generates a vector (`from,from+by,from+2*by,...`) with the last entry not extending further than `to`. In the second form the value of `by` is assumed to be 1 or -1, depending on whether `from` or `to` is larger. There are also two shortcuts for creating vectors with `by=1`:

```
> 1:8; c(1:8);
[1] 1 2 3 4 5 6 7 8
[1] 1 2 3 4 5 6 7 8
```

Exercise 3.1 Use `seq` to create the vector `v=(1 5 9 13)`, and to create a vector going from 1 to 5 in increments of 0.2 .

<code>seq(from,to,by=1)</code>	Vector of evenly-spaced values, default increment = 1
<code>seq(from,to,length)</code>	Vector of evenly-spaced values with specified endpoints and length
<code>c(u,v,...)</code>	Combine a set of numbers and/or vectors into a single vector
<code>rep(a,b)</code>	Create vector by repeating elements of a by amounts in b
<code>as.vector(x)</code>	Convert an object of some other type to a vector
<code>hist(v)</code>	Histogram plot of value in v
<code>mean(v),var(v),sd(v)</code>	Estimate of population mean, variance, and standard deviation based on data values in v
<code>cor(v,w)</code>	Correlation between two vectors

Table 3: Some important R functions for creating and working with vectors. Many of these have other optional arguments; use the help system (e.g. `?cor`) for more information.

A constant vector such as `(1,1,1,1)` can be created with `rep` function, whose basic syntax is `rep(values,lengths)`

For example,

```
> rep(3,5)
[1] 3 3 3 3 3
```

`rep(values,lengths)` can also be used with a vector of values and their associated lengths, for example

```
> rep( c(3,4),c(2,5) )
[1] 3 3 4 4 4 4 4
```

The value 3 was repeated 2 times, followed by the value 4 repeated 5 times.

Some of the main functions for creating and working with vectors are listed in Table 3. R also has many functions for creating vectors of random numbers with various distributions, that are useful in simulating stochastic models. Most of these have a number of **optional arguments**, which means in practice that you can choose to specify their value, or if you don't a default value is assumed. For example,

```
> rnorm(100)
```

yields 100 random numbers with a Normal (Gaussian) distribution, mean=0, standard deviation=1. But

```
> rnorm(100,2,5)
```

yields 100 random numbers from a Gaussian distribution with mean=2, standard deviation=5. The existence of default values for some arguments of a function is indicated by writing (for example) `rnorm(n,mu=0,sd=1)`. Since no default value is given for *n*, the user must supply one: `rnorm()` gives an error message.

Some of the functions for creating length-*n* vectors of random numbers are listed in Table 4. We will see soon some examples of using these functions to simulate models with random components to their dynamics.

Exercise 3.2 Generate a vector of 5000 random numbers from a Gaussian distribution with mean=3, standard deviation=2. Use `hist` to visualize the distribution of values, and the functions `mean`, `sd` to estimate the population mean and standard deviation from the “data” values in the vector.

3.1.2 Vector addressing

Often it is necessary to extract a specific entry or other part of a vector. This is done using subscripts, for example

<code>rnorm(n,mean=1,sd=1)</code>	Gaussian distribution(mean=mu, standard deviation=sd)
<code>runif(n,min=0,max=1)</code>	Uniform distribution on the interval (min,max)
<code>rbinom(n,size,prob)</code>	Binomial distribution with parameters #trials N =size, probability of success p =prob.
<code>rpois(n,lambda)</code>	Poisson distribution with mean=lambda
<code>rbeta(n,shape1,shape2)</code>	Beta distribution on the interval $[0,1]$ with shape parameters shape1,shape2

Table 4: Some of the main R function for generating vectors of random numbers. To create random matrices, these can be reshaped using `matrix()`. Functions to evaluate the corresponding probability distribution functions are also available. For a listing use the Help system (`?Normal`, `?Uniform`, `?Lognormal`, etc. for lists of the available functions for each distribution family).

```
> q=c(1,3,5,7,9,11); q[3]
[1] 5
```

`q[3]` extracts the third element in the vector `q`. You can also access a block of elements using the functions for vector construction, e.g. to extract the 2nd through 5th elements of `q`

```
v=q[2:5]; v
[1] 3 5 7 9
```

If you enter `v=q[seq(1,5,2)]`, what will happen? Try it and see, and make sure you understand what happened.

Extracted parts of a vector don't have to be regularly spaced. For example

```
> v=q[c(1,2,5)]; v
[1] 1 3 9
```

Addressing is also used to **set specific values within a vector**. For example,

```
> q[1]=12
```

changes the value of the first entry in `q` while leaving all the rest alone, and

```
> q[c(1,3,5)]=c(22,33,44)
```

changes the 1st, 3rd, and 5th values.

Exercise 3.3 write a **one-line** command to extract a vector consisting of the second, first, and third elements of `q` **in that order**.

Exercise 3.4 Write a script file that computes values of $y = \frac{(x-1)}{(x+1)}$ for $x = 1, 2, \dots, 10$, and plots y versus x with the points plotted and connected by a line.

Exercise 3.5 The sum of the geometric series $1 + r + r^2 + r^3 + \dots + r^n$ approaches the limit $1/(1-r)$ for $r < 1$ as $n \rightarrow \infty$. Take $r = 0.5$ and $n = 10$, and write a **one-statement** command that creates the vector $G = c(r^0, r^1, r^2, \dots, r^n)$. Compare the sum of this vector to the limiting value $1/(1-r)$. Repeat this for $n = 50$.

Vector orientation. You may be wondering if vectors in R are row vectors or column vectors (if you don't know what those are, don't worry: we'll get to it later). The answer is "both and neither". Vectors are printed out as row vectors, but if you use a vector in an operation that succeeds or fails depending on the vector's orientation, R will assume that you want the operation to succeed and will proceed as if the vector has the necessary orientation. For example, R will let you add a vector of length 5 to a 5×1 matrix or to a 1×5 matrix, in either case yielding a matrix of the same dimensions.

3.2 Matrices

3.2.1 Creating matrices

A matrix is a two-dimensional rectangular array of numbers. Matrices can be created by reading in values from a data file using `read.table`, or from a properly formatted .csv spreadsheet file using `read.csv`. Matrices of numbers can also be entered by creating a vector of the matrix entries, and then reshaping them to the desired number of rows and columns using the function `matrix`. For example

```
> X=matrix(c(1,2,3,4,5,6),2,3)
```

takes the values 1 to 6 and reshapes them into a 2 by 3 matrix.

```
> X
      [,1] [,2] [,3]
[1,]    1    3    5
[2,]    2    4    6
```

By default the values in the data vector are put into the matrix column-wise. You can change this by using the optional parameter `byrow`. For example

```
> A=matrix(1:9,3,3,byrow=T); A
      [,1] [,2] [,3]
[1,]    1    2    3
[2,]    4    5    6
[3,]    7    8    9
```

R will re-cycle through entries in the data vector, if need be, to fill out a matrix of the specified size. So for example

```
matrix(1,50,50)
```

creates a 50×50 matrix of all 1's.

Exercise 3.6 Use a command of the form `X=matrix(v,2,4)` where `v` is a data vector, to create the following matrix X

```
      [,1] [,2] [,3] [,4]
[1,]    1    1    1    1
[2,]    2    2    2    2
```

Exercise 3.7 Use `rnorm` and `matrix` to create a 5×7 matrix of Gaussian random numbers with mean 1 and standard deviation 2.

Another useful function for creating matrices is `diag`. `diag(v)` creates a square matrix with data vector `v` on its diagonal – try

<code>matrix(v,m,n)</code>	$m \times n$ matrix using the values in <code>v</code>
<code>data.entry(A)</code>	call up a spreadsheet-like interface to edit the values in <code>A</code>
<code>diag(v,n)</code>	diagonal $n \times n$ matrix with <code>v</code> on diagonal, 0 elsewhere
<code>cbind(a,b,c,...)</code>	combine compatible objects by binding them along columns
<code>rbind(a,b,c,...)</code>	combine compatible objects by binding them along rows
<code>as.matrix(x)</code>	convert an object of some other type to a matrix, if possible
<code>outer(v,w)</code>	“outer product” of vectors <code>v,w</code> : the matrix whose $(i,j)^{th}$ element is <code>v[i]*w[j]</code>
<code>iden(n)</code>	$n \times n$ identity matrix (in <code>boot</code> library)
<code>zero(n,m)</code>	$n \times m$ matrix of zeros (in <code>boot</code> library)
<code>t(x)</code>	transpose the matrix <code>x</code>
<code>dim(X)</code>	dimensions of matrix <code>X</code> . <code>dim(X)[1]=# rows</code> , <code>dim(X)[2]=# columns</code>

Table 5: Some important functions for creating and working with matrices. Many of these have additional optional arguments; use the Help system for full details.

```
diag(1:3)
```

and see what happens. `diag(v,n)` creates an $n \times n$ matrix with `v` on the diagonal, and if necessary it “recycles” through `v` to find `n` values. To see what that means, try

```
diag(1:3,5); diag(1,6)
```

to see what they create (and make sure you understand why!)

Finally, one can use the `data.entry` function. This function can only edit existing matrices, but for example (try this right now!)

```
A=matrix(0,3,4); data.entry(A)
```

will create `A` as a 3×4 matrix, and then call up a spreadsheet-like interface in which the values can be changed to whatever you need.

3.2.2 cbind and rbind

If their sizes match, vectors can be combined to form matrices, and matrices can be combined with vectors or matrices to form other matrices. The functions that do this are `cbind` and `rbind`.

`cbind` binds together columns of two objects. One thing it can do is put vectors together to form a matrix:

```
> C=cbind(1:3,4:6,5:7); C
  [,1] [,2] [,3]
[1,]  1   4   5
[2,]  2   5   6
[3,]  3   6   7
```

Remember that R interprets vectors as row or column vectors according to what you’re doing with them. Here it treats them as column vectors so that columns exist to be bound together. On the other hand,

```
> D=rbind(1:3,4:6); D
  [,1] [,2] [,3]
[1,]  1   2   3
[2,]  4   5   6
```

treats them as rows. Now we have two matrices that can be combined.

Exercise 3.8 Verify that `rbind(C,D)` works, `cbind(C,C)` works, but `cbind(C,D)` doesn't. Why not?

3.2.3 Matrix addressing

Matrix addressing is like vector addressing except that you have to specify both the row and column, or range of rows and columns. For example `q=A[2,3]` sets `q` equal to 6, which is the (2nd row, 3rd column) entry of the matrix **A** that you recently created, and

```
> A[2,2:3];
[1] 5 6
> B=A[2:3,1:2]; B
      [,1] [,2]
[1,]    4    5
[2,]    7    8
```

There is an easy shortcut to extract entire rows or columns: leave out the limits.

```
> first.row=A[1,]; first.row
[1] 1 2 3
> second.column=A[,2]; second.column;
[1] 2 5 8
```

As with vectors, addressing works in reverse to assign values to matrix entries. For example,

```
> A[1,1]=12; A
      [,1] [,2] [,3]
[1,]   12    2    3
[2,]    4    5    6
[3,]    7    8    9
```

The same can be done with blocks, rows, or columns, for example

```
> A[1,]=runif(3); A
      [,1]      [,2]      [,3]
[1,] 0.1911789 0.07919515 0.798139
[2,] 4.0000000 5.00000000 6.000000
[3,] 7.0000000 8.00000000 9.000000
```

(see Table 4 to remind yourself about `runif`).

Exercise 3.9 Write a script file to do the following. (a) Use `runif` to construct a 5×5 matrix **B** of random numbers with a uniform distribution between 0 and 1. (b) Extract from it the second row, the second column, and the 3×3 matrix of the values that are not at the margins (i.e. not in the first or last row, or first or last column). (c) Use `seq` to replace the values in the first row of **B** by 2 5 8 11 14.

3.3 Operations with Matrices and Vectors

A numerical function applied to a matrix acts element-by-element.

```
> A=matrix(c(1,4,9,16),2,2); A; sqrt(A);
[,1] [,2]
[1,]  1  9
[2,]  4 16
[,1] [,2]
[1,]  1  3
[2,]  2  4
```

The same is true for scalar multiplication and division. **Try $2*A$, $A/3$ and see what you get.**

If two matrices (or two vectors) are the same size, then you can do element-by-element addition, subtraction, multiplication, division, and exponentiation:

$A+B$, $A-B$, $A*B$, A/B , A^B

NOTE: A^B means each element in A raised to the power given by the corresponding element in B . This is **NOT** what A^B means in Matlab. So for example:

$$\text{if } C = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \text{ then } C^C = \begin{bmatrix} 1^1 & 2^2 \\ 3^3 & 4^4 \end{bmatrix}$$

Matrix-matrix and matrix-vector multiplication are indicated by the special notation `%*%`. For example,

```
> v=1:2; A%*%v
[,1]
[1,] 19
[2,] 36
```

It's essential to always remember that *element-by-element is the default*, because R's eagerness to make things work can let errors get by without warning. For example, had you forgotten to ask for matrix-vector multiplication above, R would make it work anyway:

```
A*v
[,1] [,2]
[1,]  1  9
[2,]  8 32
```

Since you inadvertently asked for element-by-element multiplication, that's what R did. It ran out of entries in v before it ran out of entries in A , so it "recycled" through the elements of v :

$$\begin{bmatrix} 1 & 9 \\ 4 & 16 \end{bmatrix} * \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 1*1 & 9*1 \\ 4*2 & 16*2 \end{bmatrix}$$

This can be a big problem because major mistakes don't get caught by R, you have to find them yourself.

The matrix algebra functions in R are front-ends for the "industry standard" numerical libraries. Some of these functions are listed in Table 6. Some of these only work on square matrices and will return an error if A is not square, in particular functions for computing eigenvalues and eivenvectors.

Some functions exist in two versions corresponding to older (LINPACK, EISPACK) and newer (BLAS,LAPACK,ATLAS) versions of these libraries. How you wind up using which is a lesson in how R works, and we leave it to the next section.

<code>outer(v,w)</code>	outer product of vectors v and w
<code>solve(A)</code>	inverse of matrix A
<code>solve(A,B)</code>	solution x of the linear system $Ax = b$ for each column b of the matrix B
<code>det(A)</code>	determinant of the matrix A
<code>norm(A)</code>	matrix norm of A (several options)
<code>eigen(A)</code>	eigenvalues and eigenvectors
<code>t(A)</code>	transpose of A
<code>exp(A)</code>	matrix exponential $\exp(A) = \sum_{n \geq 0} \frac{A^n}{n!}$ (in package <code>fMultiVar</code>)
<code>mtx.exp(A,n)</code>	efficiently compute powers of a matrix A^n (not element-by-element) (in package <code>BioDem</code>)
<code>apply(A,margin,fun)</code>	apply a function <code>fun</code> to the rows (<code>margin=1</code>) or columns (<code>margin=2</code>) of matrix A , and return all resulting values
<code>sapply(v,fun)</code>	apply a function <code>fun</code> to all elements in vector v , returning a vector of values

Table 6: Some important functions for matrix-vector numerical calculations. Many of these have additional optional arguments; use the Help system for full details

3.3.1 Eigenvalues and eigenvectors

In this section we consider only square matrices, for which eigenvalues and eigenvectors are defined. Recall that if $Aw = \lambda w$ (for A a square matrix, w a nonzero column vector, and λ a real or complex number) then λ is called an eigenvalue and w is the corresponding eigenvector of \mathbf{A} .

If v is a row-vector such that $v\mathbf{A} = \lambda v$, then v is called a *left eigenvector* of \mathbf{A} . The left eigenvalues for a matrix are the same as the (right) eigenvalues. The left eigenvectors of \mathbf{A} are the same as the right eigenvectors of the transpose $t(\mathbf{A})$.

`eigen` returns eigenvalues sorted by absolute value, with the dominant eigenvalue (meaning, the one with the largest absolute value) first. (the general definition of absolute value, which covers both real and complex numbers, is

$$|a + bi| = \sqrt{a^2 + b^2}.$$

For example,

```
A=matrix(1:9,3,3); vA=eigen(A); vA;
$values
[1] 1.611684e+01 -1.116844e+00 -9.357342e-17

$vectors
[,1]      [,2]      [,3]
[1,] -0.4645473 -0.8829060 0.4082483
[2,] -0.5707955 -0.2395204 -0.8164966
[3,] -0.6770438 0.4038651 0.4082483
```

As with the output from `lm` (you remember `lm ...`) `vA` is an *object* composed of two *components*, whose names are `values` and `vectors`. The “\$” is used to extract components of a compound object, for example `vA$values` is the `values` part of `vA`, a vector consisting of the sorted eigenvalues:

```
vA$values
[1] 1.611684e+01 -1.116844e+00 -9.357342e-17
```

The `vectors` component is a matrix whose columns are the corresponding eigenvectors, sorted in the same order as the eigenvalues. That is,

```
j=1; A%%vA$vectors[,j]-vA$values[j]*vA$vectors[,j];
[,1]
[1,] 0.000000e+00
[2,] -3.552714e-15
[3,] -3.552714e-15
```

Exercise 3.10 Verify that the output is also $(0, 0, 0)$, apart from numerical error, for $j=2$ and $j=3$. Explain in words what these calculations show.

Exercise 3.11 Enter the command `names(vA)` and see what results. From this, infer what the `names` function does. Enter the command `names(A)` and infer the meaning of the object `NULL` in R. Check your guess by using the Help system to find out what `NULL` means (`?NULL` or `help.search('Null')`).

To get the left eigenvectors of a matrix, you use `eigen` to compute the eigenvectors of its transpose, `t(A)`. So

```
vLA=eigen(t(A))$vectors
```

gets you the left eigenvectors of `A`.

Exercise 3.12 Compute `vLA[,j]%%A-vA$values[j]*vLA[,j]` to verify the last claim about left eigenvectors, for $j=1$ to 3 .

For stability analysis of differential equation models, the “dominant eigenvalue” of the Jacobian matrix is the one with the largest real part. To find this we need to extract the real parts of each eigenvalue and identify the largest one.

The help system (`?complex`) lists the R functions for working with complex numbers. The one we need here is `Re`, which extracts the real parts of complex numbers.

Use `data.entry(A)` to create the matrix

$$A = \begin{pmatrix} 3 & 0 & 0 \\ 2 & 2 & -3 \\ 0 & 3 & 1 \end{pmatrix}$$

and you should find that `eigen(A)$values` are

```
[1] 1.5+2.95804i 1.5-2.95804i 3.0+0.00000i.
```

The first two are a complex conjugate pair with absolute value `3.316625` (`abs(eigen(A)$values)` gets you the absolute values of the eigenvalues), but the third one has the largest real part.

To have R do this for you, we use the `which` function to find where the real part is maximized.

```
vA=eigen(A)$values; rmax=max(Re(vA));
j=which(Re(vA)==rmax);
lmax=Re(vA[j]); vmax=eigen(A)$vectors[,j];
```

The first line uses `max` to compute the largest real part of any eigenvalue. In the second line, `which` finds the indices at which the logical condition `(Re(vA)==rmax)` is `TRUE`, in this case $j=3$. The third line then extracts the relevant entries from the lists of eigenvalues and eigenvectors. The dominant real part will then be `Remax=Re(lmax)`.

Exercise 3.13 Try the above on `A=diag(c(3,1,3))` and see what you get for `vmax` and `Remax`. Why? [Note: the point of this exercise is that the code above for finding `lmax` and is sometimes not going to work exactly as advertised. If there is a tie for the largest real part, for example if the eigenvalues are

(3,1,3), then Remax will be `c(3,3)`, not `3`. To do the next exercise, you'll have to figure out what to do about this.]

Exercise 3.14 In this exercise we take an eigenvalue-based look at a simple (and partially re-scaled) predator-prey model:

$$\begin{aligned} dx/dt &= x(1 - x/K) - yx^q \\ dy/dt &= cyx^q - my \end{aligned} \tag{1}$$

with x = prey density, y = scaled predator density, and K, q, c, m positive constants. The interior equilibrium for this model is at

$$\bar{x} = (m/c)^{1/q}, \quad \bar{y} = (\bar{x}^{1-q})(1 - \bar{x}/K)$$

and the Jacobian matrix at a point (x, y) is

$$\begin{bmatrix} 1 - 2x/K - qyx^{q-1} & -x^q \\ cqyx^{q-1} & cx^q - m \end{bmatrix}$$

As usual with a type-II functional response ($0 < q < 1$) the model exhibits a transition from stability to cycles as K is increased (Figure 3).

(a) Write a function `domreal=function(K,q,c,m)` that computes and returns the largest real part of any eigenvalue for the Jacobian of model (1) evaluated at the interior equilibrium, as a function of the model parameters.

(b) Using your function, create a plot like that in Figure 3 panel (c), showing how the eigenvalues change as K is gradually increased from 200 to 350 with other parameters fixed at the values $q = 0.5, c = 0.1, m = 1$. (“gradually” means: compute enough values that you can plot a smooth curve as a function of K , rather than just two points connected by a line).

Figure 3: Hopf bifurcation in predator-prey model (1) with parameters $q = 0.5, c = 0.1, m = 1$. As K increases, a pair of complex conjugate eigenvalues crosses the imaginary axis in the complex plane.

3.3.2 Eigenvector scalings

For a transition matrix model, the dominant right eigenvector w (i.e. the eigenvector corresponding to the eigenvalue with largest absolute value) is the *stable stage distribution*, so we are most interested in relative proportions. To get those, $w=w/\text{sum}(w)$. The dominant left eigenvector v is the reproductive value, and it is conventional to scale those relative to the reproductive value of a newborn. If newborns are class 1: $v=v/v[1]$.

Exercise 3.15: Write a script file which applies the above to the matrices

$$A = \begin{pmatrix} 1 & -5 & 0 \\ 6 & 4 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 1 & 5 \\ 0.6 & 0 & 0 \\ 0 & 0.4 & 0.9 \end{pmatrix}$$

finding **all** the eigenvalues and then extracting the dominant one and the corresponding left and right eigenvectors. For B , use the scalings defined above.

3.3.3 Eigenvalue sensitivities and elasticities

For an $n \times n$ matrix A with entries a_{ij} , the sensitivities s_{ij} and elasticities e_{ij} of the dominant (largest absolute value) eigenvector can be computed as

$$s_{ij} = \frac{\partial \lambda}{\partial a_{ij}} = \frac{v_i w_j}{\langle v, w \rangle} \quad e_{ij} = \frac{a_{ij}}{\lambda} s_{ij} \quad (2)$$

where λ is the dominant eigenvalue, v and w are dominant left and right eigenvalues, and $\langle v, w \rangle$ is the inner product of v and w , computed in R as `sum(v*w)`. So once λ , v , and w have been found and stored as variables, it just takes some for-loops to compute the sensitivities and elasticities.

```
vA=eigen(A); lambda=vA$values[1];
w=vA$vectors[,1]; w=w/sum(w);
v=eigen(t(A))$vectors[,1]; v=v/v[1];
vdotw=sum(v*w);
s=A; n=dim(A)[1];
for(i in 1:n) {
for(j in 1:n) {
s[i,j]=v[i]*w[j]/vdotw;
}
}
e=(s*A)/lambda;
```

Note how all the elasticities are computed at once in the last line. In R that kind of “vectorized” calculation is *much* quicker than computing entries one-by-one in a loop. Even better is to use a built-in function that operates at the vector or matrix level. In this case we can use `outer` (see Table 6 or ?outer) to completely eliminate the nested do-loops:

```
vA=eigen(A); lambda=vA$values[1];
w=vA$vectors[,1]; w=w/sum(w);
v=eigen(t(A))$vectors[,1]; v=v/v[1];
s=outer(v,w)/sum(v*w);
e=(s*A)/lambda;
```

Vectorizing code to avoid or minimize loops is an important aspect of efficient R programming. The functions `apply` or `sapply` are often useful in this regard and you should look into them if you have a script that is running too slow because of loops.

Exercise 3.16 Construct the transition matrix \mathbf{A} , and then find λ , \mathbf{v} , \mathbf{w} for an age-structured model with the following survival and fecundity parameters.

Age-classes 1-6 are genuine age classes with survival probabilities $(p_1 p_2 \cdots p_6) = (0.3, 0.4, 0.5, 0.6, 0.6, 0.7)$

Note that $p_j = a_{j+1,j}$, the chance of surviving from age j to age $j + 1$, for these ages. You can create a vector \mathbf{p} with the values above and then use a for-loop to put those values into the right places in \mathbf{A} .

Age-class 7 are adults, with survival 0.9 and fecundity 12.

Results: $\lambda = 1.0419$

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 12 \\ .3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & .4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & .5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & .6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & .6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & .7 & .9 \end{pmatrix}$$

$w = (0.6303, 0.1815, 0.0697, 0.0334, 0.0193, 0.0111)$

$v = (1, 3.4729, 9.0457, 18.8487, 32.7295, 56.8328, 84.5886)$

3.4 matrix or Matrix? Classes in R

This section can be skipped for now. It will make sense if you have previous experience with object-oriented languages. Otherwise, come back to it after you've worked for a while with objects in R.

Variables and other kinds of objects in R can be assigned a *class* attribute which tells R what kind of object it is. As an example:

```
> g=matrix(0,5,5); class(g)
NULL
```

shows that the object `g` has not been assigned a class. On the other hand,

```
> library(Matrix); g=Matrix(0,5,5); class(g)
[1] "Matrix"
```

`library(Matrix)` loaded the `Matrix` library (which has some additional and higher-accuracy routines for matrix algebra). `g=Matrix(0,5,5)` created a 5-by-5 matrix of zeros, just as in the previous example, but this time the function `Matrix` assigned it a class.

Class attributes allow R functions to exist in multiple versions (called “methods”), that do different things to different classes of objects. You can list them using the `methods` function, for example

```
> methods(det);
[1] "det.default"           "det.LowerTriangular"
[3] "det.Matrix"           "det.UnitLowerTriangular"
[5] "det.UnitUpperTriangular" "det.UpperTriangular"
```

So the effect of the command `det(g)` depends on `g`'s class. If `g`'s class is `Matrix`, `det(g)` invokes `det.Matrix` to compute the determinant. If `g`'s class is `LowerTriangular` (a kind of matrix) then `det(g)` invokes `det.LowerTriangular` to compute the determinant, and so on. If `g` doesn't have a class for which a specific method exists, then `det(g)` invokes `det.default`.

This explains how R can have two sets of matrix algebra routines, as we mentioned above. The methods above for `det` are all part of the `Matrix` library (and if you try `methods(det)` without loading the `Matrix` library, you won't see them listed). With the `Matrix` library loaded, a plain old matrix will have its determinant calculated by `det.default`, while a matrix of class `Matrix` will be handled by `det.Matrix`.

The convenience of classes and methods is illustrated better by `methods(plot)`. The list that this gives you shows that R has a series of methods that generate suitable plots for a variety of classes including statistical models, time series, functions, etc. and the appropriate one is usually invoked "under the hood" without the user having to specify which one you want.

The inconvenience is that some functions require arguments of a specific class. You may then have to devote some effort to converting things from one class to another, using functions like `as.matrix`. If an error message indicates that you're in this kind of trouble, use the help system to see if a function `as.whatever` exists that can convert into the necessary class. Usually there will be one, if what you're trying to do is legitimate.

3.5 Data Frames (and more R tricks)

A common data type in R is the *data frame*, which has many of the same properties as lists, vectors and matrices. Most of what we'll do later in the course draws from our intuition about vectors and matrices. Still, data frames are ubiquitous and knowing how to use them will come in handy later on. Notably, this is the data type returned when we load data into R, so let's pull up the frog-tadpoles data.

```
> my.data = read.csv(file=file.choose(), header=F);
> names(my.data) = c("Frogs", "Tadpoles");
```

We can query what type of object `my.data` is using the commands `mode`, `typeof`, which tell us it's of the generic type `list`. We can get more specific using `class`, or any of the many `is.` (data type) commands:

```
> class(my.data);
> is.matrix(my.data);
> is.data.frame(my.data);
```

To see other such function, use the autocomplete capabilities in R. Type the start of a function name then hit tab twice to show a list of possibilities:

```
> is.<TAB><TAB>
is.array          is.atomic          is.call            is.character       ...
is.double         is.element         is.empty.model    is.environment     ...
...
```

In short, data frames are most useful because they can have columns of different data types:

```
> data.frame(chars=letters[1:10], ints=90:99, logicals=rep(c(TRUE,FALSE),5));
```

3.5.1 Data frame addressing

Data frames can be treated just like matrices, addressing by row and column:

```
> my.data;
> my.data[2:4,]
  Frogs Tadpoles
2   1.3 2.876231
3   1.7 3.062528
4   1.8 3.707180
> my.data[2:4,2]
[1] 2.876231 3.062528 3.707180
```

Data frames can also have rows and columns indicated by their names, using either square brackets or the special character `$`:

```
> names(my.data)
[1] "Frogs" "Tadpoles"
> my.data$Frogs;
```

<code>data.frame(u,v,...)</code>	combines columns u , v into a data frame
<code>names(x)</code>	access the column names in the data frame x
<code>as.data.frame(x)</code>	convert an object of some other type to a data frame, if possible
<code>attach(x)</code>	include columns of x in the workspace
<code>head(x)</code>	view the first few rows of x
<code>tail(x)</code>	view the last few rows of x

Table 7: More functions for creating and working with data frames. Also see the functions for matrices like `cbind`. See the help for details.

```
[1] 1.1 1.3 1.7 1.8 1.9 2.1 2.3 ...
> my.data$Tadpoles;
[1] 2.036982 2.876231 3.062528 3.707180 ...
> my.data["Frogs"];
  Frogs
1   1.1
2   1.3
...
> my.data[3:5,"Tadpoles"];
```

Exercise 3.17 Use the `data.frame()` and `names()` functions to make the following data frame

```
      sex weight
1     M   135
2     F   106
3     M   164
4     F   127
```

What happens if you use `as.matrix()` to convert it to a different data type? What about with `as.vector()`?

3.5.2 More on vector, matrix and data frame addressing

One somewhat advanced (and R specific) way of pulling out specific elements of a vector (and rows or columns of a matrix or data frame) is using a vector of logicals (`TRUE`, `FALSE` statements). Indexing with a vector of `TRUE/FALSE` values, only the elements with a `TRUE` are returned.

```
> set.seed(101)
> x=runif(9); x
[1] 0.372 0.0438 0.709 0.657 0.249 0.300 0.584 0.333 0.622
> x[rep(c(T,F,F),3)]
[1] 0.372 0.657 0.584
```

Thus the equivalent to returning “all x less than 0.6” is accomplished by

```
> x<0.6
[1] TRUE TRUE FALSE FALSE TRUE TRUE TRUE TRUE FALSE
> x[x<0.6]
[1] 0.37219838 0.04382482 0.24985572 0.30005483 0.58486663 0.33346714
```

Exercise 3.18 Use the above and the frog-tadpole data to determine which in rows there are more than twice as many tadpoles as frogs (i.e. $2 * \text{Frogs} < \text{Tadpoles}$). Can you create a third column (e.g. `my.data$Over`) indicating this outcome for each row?

Additional Exercises: Vectors, Matrices, Data Frames

Exercise 3.19 Before typing in the commands, write down the matrices *that you think* will be returned by `matrix(1:4)`, `matrix(1:4,2,2)`, and `matrix(1:4,2,2,byrow=F)`. After confirming your answers with R, see the help for `matrix()` to describe any discrepancies or confirm your correct reasoning.

Exercise 3.20 Use `diag()` and then `data.entry()` to create the following matrix A.

```
> A
      var1 var2 var3 var4
[1,]    1    0    5    7
[2,]    0    2    6    8
[3,]    0    0    3    0
[4,]    0    0    0    4
```

Replace the four non-zero values in the upper right corner of the matrix

```
> A[1:2 , 3:4]
      var3 var4
[1,]    5    7
[2,]    6    8
```

with the 2x2 matrix given by `matrix(1:4,2,2,byrow=TRUE)`.

Exercise 3.21 Frequently, a column or two of a large data frame is used to define a new object. Depending on the data type we want for this new object (e.g. a vector, matrix or data frame), we can extract the columns (or rows) in different ways. Using the frog-tadpole data, and recalling that `my.data` is a data frame, we can extract the first column of data using either: `my.frogs = my.data[,1]`, `my.frogs = my.data$Frogs`, `my.frogs = my.data["Frogs"]`, or `my.frogs = my.data[[1]]`. Try each, and describe how these differ (or are the same) using the functions like `mode`, `class`, `is.matrix`, `is.data.frame`, etc.

4 Iteration (“Looping”)

Loops make it easy to do the same operation over and over again, for example:

- Making population forecasts 1 year ahead, then 2 years ahead, then 3, etc.
- Simulating a model multiple times, with different values for one of the parameters.

There are two kinds of loops in R: **for** loops, and **while** loops. A **for** loop runs for a specified number of steps, and a **while** loop runs until a certain condition is met.

4.1 For-loops

The **for** loops are written as

```
for (var in seq) {
  commands
}
```

The dummy variable **var** is sequentially assigned the values in the list **seq**, each time executing the code between braces { }. Here’s an example (file **Loop1.R**):

```
# initial population size
initsize=4;

# create vector to hold results and store initial size
popsize=rep(0,10); popsize[1]=initsize;

# calculate population size at times 2 through 10, write to Command Window
for (n in 2:10) {
  popsize[n]=2*popsize[n-1];
  x=log(popsize[n]);
  cat(n,x,"\n");
}
plot(1:10,popsize,type="l");
```

The first time through the loop, $n=2$. The second time through, $n=3$. When it reaches $n=10$, the for-loop is finished and R starts executing any commands that occur after the end of the loop. The result is a table of the log population size in generations 2 through 10.

Note also the **cat** function (short for “concatenate”) for printing results to the console window. **cat** converts its arguments to character strings, concatenates them, and then prints them. The “**\n**” argument is a line-feed character (as in the **C** language) so that each (n,x) pair is put on a separate line.

Several **for** loops can be nested within each other, which is needed for working with matrices as in the example below. It is important to notice that the second loop is **completely** within the first. Loops must be either **nested** (one completely inside the other) or **sequential** (one starts after the previous one ends).

```
A=matrix(0,3,3);          (1)
```

```

for (row in 1:3) {           (2)
  for (col in 1:3) {       (3)
    A[row,col]=row*col    (4)
  }                         (5)
}                            (6)
A;                          (7)

```

Type or copy this into a script file and run it; the result should be

```

      [,1] [,2] [,3]
[1,]    1    2    3
[2,]    2    4    6
[3,]    3    6    9

```

Line 1 creates A as a matrix of all zeros - this is an easy way to create a matrix of whatever size you need, which can then be filled in with meaningful values as your program runs. Then two nested loops are used to fill in the entries. Line 2 starts a loop over the rows of A, and immediately in line 3 a loop over the columns is started. To fill in the matrix we need to consider all possible values for the pair (row, col). So for row=1, we need to consider col=1,2,3. Then for row=2 we also need to consider col=1,2,3, and the same for row=3. That’s what the nested for-loops accomplish. For row=1 (as requested in line 2), the loop in lines 3-5 is executed until it ends. Then we get to the end in line 6, at which point the loop in line 2 moves on to row=2, and so on.

Nested loops also let us automate the process of running a simulation many times, for example with different parameters or to look at the average over many runs of a stochastic model. For example (**Loop2.R**),

```

p=rep(0,5);                 (1)
for (init in c(1,5,9)){    (2)
  p[1]=init;               (3)
  for (n in 2:5) {         (4)
    p[n]=2*p[n-1]         (5)
    cat(init,n,p[n],"\n"); (6)
  }                         (7)
}                            (8)

```

Line 1 creates the vector p. Line 2 starts a loop over initial population sizes Lines 4-7 does a “population growth” simulation Line 8 then closes the loop over initial sizes

The result when you run **Loop2.R** is that the “population growth” calculation is done repeatedly, for a series of values of the initial population size. To make the output a bit nicer we can add some headings as the program runs - source **Loop3.R** and then look at the file to see how the formatting was done.

If this discussion of looping doesn’t make sense to you, **stop now and ask for some help!** Loops are essential from here on out.

Exercise 4.1: Imagine that while doing fieldwork in some distant land you and your assistant have picked up a parasite that grows exponentially until treated. Your case is more severe than your assistant’s: on return to Ithaca there are 400 of them in you, and only 120 in your assistant. However, your field-hardened immune system is more effective. In your body the number of parasites grows by 10 percent each day, while in your assistant’s it increases by 20 percent each day. That is, after your return to Ithaca your parasite load $n(j)$ grows according to the rule $n[j+1]=1.1*n[j]$ where j is time in days, and your assistant’s parasite load grows according to the rule $m[j+1]=1.2*m[j]$.

Write a script file **Parasite1.R** that uses a for-loop to compute the number of parasites in your body and your assistant’s over the next 30 days, and draws a single plot of both on log-scale (i.e. $\log(n(j))$ and $\log(m(j))$ versus time for $j=1$ to 30 days). **Save the script!** You’ll be using it later, as the starting point for some other exercises.

Exercise 4.2: Write a script file that uses for-loops to create the following 5×5 matrix A. Think first: do you want to use nested loops, or sequential?

$$\begin{matrix} 0 & 1 & 2 & 3 & 4 \\ 0.1 & 0 & 0 & 0 & 0 \\ 0 & 0.2 & 0 & 0 & 0 \\ 0 & 0 & 0.3 & 0 & 0 \\ 0 & 0 & 0 & 0.4 & 0 \end{matrix}$$

Exercise 4.3 Write a for loop that fills vector X with the first 100 Fibonacci numbers starting at 0.

Exercise 4.4 Write a script file that uses a for-loop to calculate solutions of the difference equation model

$$N(j+1) = r(j)N(j)/(1 + N(j)), \quad N(1) = 1$$

up to $j = 13$, where $r(j) = 2e^{-0.2j}$. Remember that in R, e^x is computed using the `exp` function. Write your script so that all values of $r(j)$ are computed and stored in a vector before the start of the for-loop, and have your script plot the solution as a graph of $N(j)$ versus j with the values plotted as points and connected by lines.

Exercise 4.5 Modify your script file from the previous exercise so that it reads a list of 12 positive numbers from a text file named `r.txt` into an vector named `r`, and then uses a for-loop to calculate the values of $N(j)$. You can use the R script editor or any other text editor to create `r.txt` and put into it any *positive* numbers that you like. This would be a good occasion to use `?scan` and `?read.table` to remind yourself about these functions for reading data into R.

Exercise 4.6 Use a for loop and the `Sys.sleep()` function to make an animated particle diffusion cartoon described by the *pseudocode* below:

```
N=500 particles
x,y = coordinate vectors
      initialize from normal distribution, mean 0.5, variance (ahem) 0.0025
for 100 time steps {
  update the coordinates by adding Normal(0,0.01) noise to x,y
  plot the points using pch=19, xlim=c(0,1), and ylim=c(0,1)
  pause for 0.05sec
}
```

<code>x < y</code>	less than
<code>x > y</code>	greater than
<code>x <= y</code>	less than or equal to
<code>x >= y</code>	greater than or equal to
<code>x == y</code>	equal to
<code>x != y</code>	not equal to

Table 8: Some comparison operators in R. Use `?Comparison` to learn more.

4.2 While-loops

A `while` loop lets an iteration continue until some condition is satisfied. For example, we can solve a model until some variable reaches a threshold. The format is

```
while(condition){
  commands
}
```

The loop repeats as long as the condition remains true. **Loop4.R** contains an example similar to the for-loop example; source it to get a graph of population sizes over time. A few things to notice about the program:

1. Although the condition in the while loop said `while(popsize<1000)` the last population value was > 1000 . That’s because the loop condition is checked **before** the commands in the loop are executed. When the population size was 640 in generation 6, the condition was satisfied so the commands were executed again. After that the population size is 1280, so the loop is finished and the program moves on to statements following the loop.
2. Since we don’t know in advance how many iterations are needed, we couldn’t create in advance a vector to hold all the results. Instead, a vector of results was constructed by starting with the initial population size and appending each new value as it is calculated. .
3. When the loop ends and we want to plot the results, the “y-values” are `popsize`, and the x values need to be `0:something`. To find “something”, the `length` function is used to find the length of `popsize`.

Within a while-loop it is often helpful to have a **counter** variable that keeps track of how many times the loop has been executed. In the following code, the counter variable is `n`:

```
n=1;
while(condition) {
  commands
  n=n+1;
}
```

The result is that `n=1` is true while the `commands` (whatever they are) are being executed for the first time. Afterward `n` is set to 2, and this remains true during the second time that the commands are executed, and so on. One use of counters is to store a series of results in a vector or matrix: on the n^{th} time through the commands, put the results in the n^{th} entry of the vector, n^{th} row of the matrix, etc.

The conditions controlling a **while** loop are built up from operators that compare two variables (Table 8). These operators return a logical value of `TRUE` or `FALSE`. For example, try:

```
> a=1; b=3; c=a<b; d=(a>b); c; d;
```

The parentheses around $(a>b)$ are optional but can be used to improve readability in script files.

Warning! $x=y$ and $x==y$ are two completely different things. The first is an *assignment*, in which x is assigned a new value. The second is a *comparison*.

When we compare two vectors or matrices of the same size, or compare a number with a vector or matrix, comparisons are done element-by-element. For example,

```
> x=1:5; b=(x<=3); b
[1] TRUE TRUE TRUE FALSE FALSE
```

R also does arithmetic on logical values, treating TRUE as 1 and FALSE as 0. So `sum(b)` returns the value 3, telling us that 3 entries of x satisfied the condition $(x \leq 3)$. This is useful for running multiple simulations and seeing how often one outcome occurred rather than another.

Exercise 4.7 Write a script file **Parasite2.R** that uses a while-loop to compute the number of parasites in your body and your assistant’s so long as you are sicker than your assistant (i.e. so long as $n > m$) and stops when your assistant is sicker than you. Use a copy of **Parasite1.R** as your starting point.

Exercise 4.8 Rewrite the for loop in the following code using a while loop and a counter variable j :

```
# Simulate something close to Brownian Motion
set.seed(3);
Year = seq(1980,2009,by=0.01);
Value = cumsum(rnorm(length(Year)));
Value = Value - min(0,min(Value))+1;

# Plot all the data
par(ask = TRUE);
plot(Year, Value, type="l", main=paste("Years",1980,"to",2008));

# Plot each half-decade
for(j in seq(1980,2000,by=5)) {
  plot(Year, Value, type="l", lwd=3, xlim=c(j,j+5), main=paste("Years",j,"to",j+5));
}
```

4.2.1 Logical operators

Sometimes we need to make decisions based on several different criteria: is $x > 3$ and also $y > 5$?. For these, **logical operators** are used to make and combine multiple comparisons:

!	Negation
& &&	AND
	OR

OR is **non-exclusive**, meaning that $x|y$ is true if x is true, if y is true, or if both x and y are true. For example:

```
>> a=c(1,2,3,4); b=c(1,1,5,5); (a<b)&(a>3); (a<b)|(a>3);
```

The two forms of AND and OR differ in how they handle vectors. The shorter one does element-by-element comparisons; the longer one only looks at the first element in each vector.

An alternative to $(x==y)$ is the **identical** function. `identical(x,y)` returns TRUE if x and y are exactly the same, else FALSE. For example, if x and y are vectors, then $x==y$ will return a vector of

values for element-by-element comparisons, while `identical(x,y)` returns a single value: TRUE if each entry in `x` equals the corresponding entry in `y`, otherwise FALSE. You can also use `all(x==y)`, which takes the element-by-element vector returned by `x==y` and returns TRUE if all are TRUE, FALSE otherwise. You can use `?Logical` to read more about logical operators.

Exercise 4.9 Use the `identical` function to construct a one-line command that returns TRUE if each entry in a vector `rnorm(5)` is positive, and otherwise returns FALSE. **Hint:** `rep` also works on logical variables, so `rep(TRUE,5)` returns the vector `(TRUE,TRUE,TRUE,TRUE,TRUE)`.

Exercise 4.10 Construct a *different* one-line command that returns TRUE if each entry in a vector `rnorm(5)` is positive, and otherwise returns FALSE. This time use the fact that R does arithmetic on logical values. (Note: the point of this and the previous exercise is to emphasize ways of *vectorizing* operations – avoiding the use of loops, which are slow, when you could express the same computation as a single operation on a vector or matrix.)

Exercise 4.11 R has two lists `letters` and `LETTERS` that contain lower case and upper case letters, respectively. The function `sample(x,n)` takes a list `x` and return `n` elements chosen randomly from that list (with or without replacement). Write a `while` loop that samples 3 `LETTERS` with replacement, and does so until this random word equals `c("E", "E", "B")`. Use a counter variable to track the number of loops, and don't forget to initialize the `word`. **Warning!** This should only take a few seconds to run! If the while loop doesn't want to stop, the ESC key will stop the current calculation.

Exercise 4.12 Write a `for` loop that repeats the previous `while` loop 100 times and stores the number of guesses needed to match the word. Plot a histogram of the number of guesses, and discuss what distribution these numbers should follow.

4.3 Iteration alternatives in R: flavors of `apply()`

Our goal as programmers in R is to try write code that takes advantage of what R has under the hood. It’s faster, takes less code (less room for error!) and makes your code easy for others to read and understand. One way we do this is to use vectors and matrices instead of an excess of `for` and `while` loops. An additional set of R specific tools to avoid unnecessary element-by-element code, are the set of functions which include `apply()`, `lapply()`, `sapply()`, and `tapply()`. They each take at least two arguments: an object (usually a matrix or data frame) `X`, and a function which is then *applied* to the rows, columns or individual elements of `X`. The result is then returned as a list, matrix or data frame. See the help for these functions for details.

To illustrate their use, here are a couple of examples.

Example 1: `sapply()` vs. `for()`

```
squareplusone = function(x) { return(1 + x^2); }
X = seq(0,10,by=2);
Y = rep(NA,length(X));

# This for loop...
for (j in 1:length(X) ) {
  Y[j] = squareplusone(X[j]);
};
Y

# ... does the same thing as this sapply() command.
Y = sapply(X,squareplusone);
Y
```

Example 2: Computing column means for a matrix

```
X = matrix(rnorm(60,c(10,20,30)),20,3,byrow=T); X
Y = apply(X,2,mean); # 2nd argument: take the mean of each 1=row, 2=column.
Y
```

Exercise 4.13 Modify the `apply()` command in the Example 2 above so that it returns the row sums in a vector.

Exercise 4.14 Write a for loop that yields the same result as `Y = apply(X,1,sd)`;

Exercise 4.15 Define a function `lessmean()` that takes an vector `z` and returns the mean of `z` after chopping off the decimal part of each number in `z` (hint: `floor()`). Modify the `apply()` command in Example 2 above so that it computes the `lessmean()` values of each column of `X`.

5 Branching: using if and else

Returning now to the comparison operators, we often use “rules” for model simulation or data processing that depend on the values of certain R objects. The `if/else` statements lets us do this; the basic format is

```
if(condition) {
  do some commands
}else{
  do some other commands
}
```

If `condition` is `TRUE` the first block of code is run, otherwise the second block of code gets called.

An `if` block can be set up in other ways, but the layout above, with the `}else{` line to separate the two sets of commands, can always be used. If the “else” is to do nothing, you can always just leave it out.

Exercise 5.1 Look at and source `Branch1.R` to see an `if` statement which makes the population growth rate depend on the current population size.

Exercise 5.2 Modify a copy of the `Parasite1.R` script so that there is random variation in parasite success. Specifically, on “bad days” the parasites increase by 10%, while on “good days” they are beaten down by your immune system and they go down by 10%; for your assistant the variation is $\pm 20\%$. That is,

$$\begin{aligned} \text{Bad days: } n(j+1) &= 1.1n(j), & m(j+1) &= 1.2m(j) \\ \text{Good days: } n(j+1) &= 0.9n(j), & m(j+1) &= 0.8m(j) \end{aligned}$$

Do this by using `runif(1)` and an `if` statement to “toss a coin” each day: if the random value produced by `runif` for that day is < 0.25 it’s a good day, and otherwise it’s bad. Be sure that your script does one new coin toss for each new day.

5.1 Nested if statements

More complicated decisions can be built up by nesting one `if` block within another. `Branch1.R` can be modified to use nested `if` and `else` statements to have population growth tail off in several steps as the population size increases:

```
for (i in 1:50) { (1)
  if(popnow<250){ (2)
    popnow=popnow*2; (3)
  }else{ (4)
    if(popnow<500){ (5)
      popnow=popnow*1.5 (6)
    }else{ (7)
      popnow=popnow*0.95 (8)
    } (9)
  } (10)
  popsize=c(popsize,popnow); (11)
} (12)
```

What does this accomplish?

- If `popnow` is still < 250 , then line 3 is executed growth by a factor of 2 occurs. Since the `if` condition was satisfied, the entire `else` block (line numbers 5-10 above) isn't looked at; R jumps line to line (11) and continues from there.
- If `popnow` is not < 250 , R moves on to the `else` on line 4, and immediately encounters the `if` on line 5.
- If `popnow` is < 500 the growth factor of 1.5 applies. Then R jumps to line (11) and continues from there.
- If neither of the two `if` conditions is satisfied, the final `else` block is executed and population declines by 5% instead of growing.

Alternatively, nested `else-if` statements can also be written as

```
if(condition1) {
  do something
} else if(condition2) {
  do something different
} else if(condition3) {
  do something completely different
} else {
  do something else
}
```

Exercise 5.3 Modify **Branch1.R** to include the nested `if` statements (1)-(10) above. Once that works, then rewrite it using the alternative format using `... } else if() {...` described above.

Exercise 5.4 Use nested `if`'s to write a script that draws one random number U between 0 and 1 using `runif(1)` and then writes to the console window “Small”, “Medium”, or “Large” depending on whether U is $\leq 1/3$, between $1/3$ and $2/3$, or $\geq 2/3$.

Exercise 5.5 Modify the script from the previous exercise and define a function `Magic8()` that takes a question (a string) as an argument and returns a random answer of “yes”, “no” or “maybe.”

5.2 Functions `ifelse()` and `switch()`

Sometimes you may wish to do something as simple as define one variable in a way that depends on the value of another variable. For example,

```
if(x==1) {
  y="a";
} else {
  y="b";
}
```

This can often be done using either `ifelse()` or `switch()`. The first of these two functions evaluates an expression (it's first argument) and returns one of two values depending on whether or not that expression is true or false.

```
x = round(runif(1)); # x = a 0,1 coin toss
y = ifelse(x==1, "x is 1", "sorry, x wasn't 1"); y;
```

When more than a simple TRUE/FALSE decision determines the value to return, the `switch()` function works in a similar way (see the help for important details).

```
x = sample(c("a","b","c","d"),1); # pick a random letter
y = ifelse(x==1, "x is 1", "sorry, x wasn't 1"); y;
```

The `switch()` function will evaluate an expression followed by n arguments. It returns the argument corresponding to the number returned by the expression:

```
x = sample(1:5,1);
y = switch(x, "first","second","third","fourth","fifth"); x; y;
```

The `switch()` function also can take character values and return a corresponding value specified in the other arguments

```
x = sample(c("a","b","c","d"),1); # pick a random letter
y = switch(x, a="A", b="B", c="C", d="D"); x; y;
```

Exercise 5.6 Using a random row of the data in `FakeDiseaseData.csv` (see `?sample`) use the `switch()` function to return "Male", "Female" or "Unknown" based on the value of `Name` in that row.

Exercise 5.7 Using the data from the previous exercise, write a `for` loop that adds a third column `Sex` to the data frame. Do this first using nested `if-else` statements, then create a second script that uses the `switch()` function.

6 Writing your own functions

Functions (often called subroutines in other programming languages) allow you to break a program into subunits. Each function is an independent little program, performing a few related tasks and returning the results. This makes complex problems easier to program, and makes it easier to see the logical flow of a large program. Each function can be written and tested independently, before you try to put all the pieces together.

Also, many R functions for simulation and data analysis require that you specify your model in the form of a function – for example, a system of differential equations that you want to solve numerically, or a nonlinear model that you want to fit to experimental data. The R function (for solving differential equations, doing nonlinear least squares, etc.) is then “told” the name of your function, and does its job on your particular model.

The basic syntax for creating a function is as follows. Suppose [for the sake of an example] you want a function `mysquare` that produces sums of squares: given vectors `v` and `w`, it returns a vector consisting of the element-by-element sums of the squares of the elements in the two vectors. The syntax is then:

```
mysquare=function(v,w) {
  u=v^2+w^2;
  return(u)
}
```

This code adds `mysquare` as an R command, just like `sin` or `log`. The variable `u` is *internal* to the function; if you use `mysquare` in a program, the program won’t “know” the value of `u`. You can save some typing by computing the final value within the return statement:

```
mysquare=function(v,w) {return(v^2+w^2)}
```

Exercise 6.1 Type the above into a script file and run it, and then do `q=mysquare(1:4,1:4)`; `q` in the console window.

Schematically, a function is defined by a code block like this:

```
function.name=function(argument1,argument2,...) {
  command;
  command;
  ...
  command;
  return(value)
}
```

Functions can return several different values, by combining them into a list with named parts.

```
mysquare2=function(v,w) {
  q=v^2; r=w^2
  return(list(v.squared=q,w.squared=r))
}
```

You can then extract the components in the usual way.

```
> x=mysquare2(1:4,2:5); names(x);
```

```
[1] "v.squared" "w.squared"
> x$v.squared
[1] 1 4 9 16
```

Functions can be placed **anywhere** in a script file. Once the code defining the function has been executed within a session, the new function can be treated like any other R command. However, **user-defined functions “vanish” when you end a session.** To use them again in another session, the function code needs to be run again. Alternatively, you can set things up (on your R at home) so that functions you use consistently are automatically loaded whenever R starts; the next subsection describes how.

Exercise 6.2 Write a function `stats(v)` that takes as input a single vector, and returns a list with named components `average` (mean of the values in the vector), and `variance` (population variance estimated from the values in the vector, using `var`). Verify that once you’ve sourced the function definition, you get

```
> stats(1:21);
$average
[1] 11
$variance
[1] 38.5
```

Exercise 6.3 Write a function to compute a forager’s expected rate of energy gain $R(t_1, t_2)$ in a Patch Model with two patch types, travel time $T = 3$, 70% patches of type 1 with gain function $g_1(t) = 2t^{0.5}$, and 30% of type 2 with $g_2(t) = t^{0.7}$. Recall that the gain rate as a function of the GUTs t_i in a Patch Model with multiple patch types is

$$R = \frac{\sum_i P_i g_i(t_i)}{T + \sum_i P_i t_i}$$

where P_i is the fraction of type- i patches. Save this script as **TwoPatchRate.R**, we’ll be using it later.

Exercise 6.4 This exercise is about using a function in a script to simulate the random population growth model

$$n(t+1) = \lambda(t)n(t), n(0) = 1. \quad (3)$$

(a) Write a function `new.pop(nt)` whose input argument `nt` is a number representing population size n in year t , and which returns the number $\lambda \times nt$ where $\lambda = e^Z$ and Z is a random number having a normal distribution with `mean=0.05`, `sd=0.5`. Z should be generated by `rnorm` within the function, so that a new value of Z is generated each time the function is called.

(b) Write a script that uses the `new.pop` function to simulate the model (3) from time $t = 0$ to $t = 50$, and then plots $n(t)$ over time.

Exercise 6.5 (a) Modify your script from the last exercise so that the input to `new.pop` can be a vector rather than a single number, say $nt = (n_1, n_2, n_3, \dots, n_d)$, and the returned value is the vector with components $n_i \lambda_i(t)$ with each λ_i having the distribution for λ specified in the last exercise. Do this in such a way that the function does not use any loops (hint: remember what `u*v` is when `u` and `v` are equal-size vectors), and that `new.pop` can use the `length` function to find out how long `nt` is).

(b) Having done this, you can now modify your script so that it simulates many populations that each follow the random growth model (3), i.e.

$$n_i(t+1) = \lambda_i(t)n_i(t), n_i(0) = 1, \quad i = 1, 2, \dots, d$$

using a single loop on time t – which is much faster than a nested loop over time and over populations. Use `matplot` to display the results for $t = 0, 1, \dots, 50$ and $d = 20$ replicate populations. [Hint: set up `nt` as a matrix with d columns, and 1’s in the first row. One call to `new.pop` with the first row as input, returns values for the second row: `nt[2,]=new.pop(nt[1,])`. And so on, as often as needed).

7 Solving differential equations

In addition to basic programming, R includes many functions that make it relatively simple to do some complicated things, relative to the effort required in a compiled language such C or fortran. A prime example is finding numerical solutions for a system of differential equations

$$dx/dt = f(t, x) \quad (4)$$

Here t is time, and x is the state vector of the system, i.e.

$$x(t) = (x_1(t), x_2(t), \dots, x_n(t))$$

where the $x_i(t)$ are the state variables of the model.

The scripts mentioned below use function for computing numerical solutions to ODEs found in the R package **odesolve**. However, this package has been replaced by the improved version, **deSolve**. This updated package (i.e., the one you should use!) includes an `ode()` function, which is a wrapper around the `lsoda` function mentioned below, and others like it. I encourage you to go through the examples below, and as an exercise replace the use of **odesolve** with **deSolve** and `ode()` instead. For more information, see `?ode` and “Solving Differential Equations in R” by Soetaert, Petzoldt and Setzer. Discussion of which solvers to use instead of `lsoda`, and when, is beyond the scope of this document.

When using **odesolve** or **deSolve** packages, the first step is to write an R function to evaluate the right hand side of your ODE, i.e., f , in eqn. (4). For example, here is an example of the Lotka-Volterra competition equations (see the example file **SolveLotka.R**):

$$\begin{aligned} dx_1/dt &= x_1(2 - x_1 - ax_2) \\ dx_2/dt &= x_2(3 - x_2 - bx_1) \end{aligned} \quad (5)$$

and here is the function that you would write for it:

```
lotka=function(t,x,parms) {
  a=parms[1]; b=parms[2];
  xdot=rep(0,2);
  xdot[1]=x[1]*(2-x[1]-a*x[2]);
  xdot[2]=x[2]*(3-x[2]-b*x[1]);
  return(list(xdot));
}
```

There’s a lot to digest in this function, so here are a few things to note:

1. The function must have input arguments (`t,x,parms`), even if only `x` is used to compute the derivative. These are a time value `t`, a state variable vector `x`, and a parameter value list `parms`, but these can be named whatever you’d like (e.g., `(ts,yvals,parms)` would also work).
2. `parms` is a vector of parameter values for function. This allows you to write a function with “free” parameters, so that you can see how solutions change as parameters are varied, without having to re-write the function for each new parameter set. It also simplifies the process of fitting differential equations to data (we’ll be doing this soon).
3. The derivative has to be returned as a list. There’s a good reason for this; if you’re curious and have *way* too much free time on your hands (you’ve been warned!), `?odesolve::lsoda` gives the explanation.

The second step is to use an R function that implements an algorithm for numerical solution of differential equations. These are in the **odesolve** package, which has to be loaded (at the command line or at the top of a script file) by

```
library(odesolve).
```

Note: Replace **odesolve** with **deSolve** in the scripts, if needed, as **odesolve** may some day be removed from the package repository.

One “basic” solver is **rk4** which implements the 4th-order Runge Kutta method with a fixed time step. The format is

```
out=rk4(x0,times,func,parms)
```

- **x0** is the initial value of the state variable vector **x** at time **times[1]**
- **times** is a vector of the time values for which you want $x(t)$ values
- **func** is the function specifying the model (such as the **lotka** function above)
- **parms** is the vector of parameter values passed to **func**

So here is an example using our **lotka** function:

```
x0=c(2,1);
times=(0:200)/10;
parms=c(0.5,0.5);
out=rk4(x0,times,lotka,parms)
matplot(out[,1],out[,2:3],type="l",ylim=c(0,3));
```

As the last line indicates, **rk4** returns a matrix in which the first column gives the times at which solution values were obtained, and the remaining columns give the (approximate) state vector values.

You can do the same more compactly once you get the hang of it:

```
out=rk4(c(2,1),(0:200)/10,lotka,c(0.5,0.5))
```

In the line above, the values of the input arguments are specified within the call to **rk4**. When doing a function call this way, the arguments have to occur in the order that the function expects. For example, try switching the order of the 2nd and 3rd arguments:

```
out=rk4(c(2,1),lotka,(0:200)/10,c(0.5,0.5))
```

The result is an error message, because **rk4** is expecting a numeric vector as its second argument, and it gets a function name instead. If you supply the names of arguments, then they can go in any order, for example:

```
out=rk4(y=c(2,1),func=lotka,times=(0:200)/10,parms=c(0.5,0.5))
```

7.1 Always use **lsoda**! Except when you shouldn't...

The RK4 method has limitations, so a more reliable method to use is **lsoda** (although, see `?ode` after loading the **deSolve** package for alternatives). This general-purpose differential equation solver was developed at Lawrence Livermore National Laboratory and automatically switches between stiff and non-stiff methods (if that terminology means anything to you) to improve numerical accuracy. The full range of possible arguments to **lsoda** are

```
lsoda(y, times, func, parms, rtol=1e-06, atol=1e-06, tcrit=NULL,
      jacfunc=NULL, verbose=FALSE, dllname=NULL, hmin=0, hmax=Inf)
```

Don't panic! Defaults are provided for everything except for the case-specific arguments required by `rk4`, so `lsoda` can be called just like `rk4`:

```
out=lsoda(x0,times,lotka,parms)
matplot(out[,1],out[,2:3],type="l",ylim=c(0,3));
```

For the most part you can get away with this, so for now we will.

One key reason for using `lsoda` rather than `rk4` is *stiffness*. Differential equations are called stiff if they have some variables or combinations of variables changing much faster than others. Stiff systems require special techniques and are harder to solve than non-stiff systems. The `lsoda` solver monitors the system that it is solving for signs of stiffness, and automatically switches to a stiff-system solver when necessary. Many biological models are at least mildly stiff, so for real work you should *always* use `lsoda` rather than `rk4`. The only time to try `rk4` is that if `lsoda` fails on your problem (returning an error message rather than a solution matrix), you may get a clue as to the reason by trying `rk4` with a very small time step and seeing how the solutions behave (e.g., does a state variable blow up to infinity in finite time?).

Exercise 7.1 Write a script file that uses `lsoda` to replicate the results in Figure 3.7 of Bulmer chapter 3, for the classical Rosenzweig-MacArthur predator-prey model (n_1 is the prey, n_2 the predator, and we write the model in the usual form)

$$\begin{aligned} dn_1/dt &= r_1 n_1 (1 - n_1/K_1) - n_2 \frac{a_1 n_1}{B + n_1} \\ dn_2/dt &= n_2 \frac{a_2 n_1}{B + n_1} - r_2 n_2 \end{aligned} \quad (6)$$

and parameter values $r_1 = r_2 = 1, a_1 = a_2 = 2, B = 200$ with initial values $n_1(0) = 300, n_2(0) = 50$. The result to be replicated is that for $K_1 = 500$ predator and prey converge to an equilibrium, while for $K_1 = 650$ they settle into a steady pattern of cyclic oscillations. To graphically show what happens in each case, have your script file solve the model from $t = 0$ to 100, and plot the densities of predator and prey populations as a function of time.

Exercise 7.2 Modify your script file from the previous exercise to incorporate **predator switching** in the form of a type-III functional response. Specifically,

(a) add a parameter $q > 1$ affecting how the predator responds to changes in prey density:

$$\begin{aligned} dn_1/dt &= r_1 n_1 (1 - n_1/K_1) - n_2 \frac{a_1 n_1^q}{B^q + n_1^q} \\ dn_2/dt &= n_2 \frac{a_2 n_1^q}{B^q + n_1^q} - r_2 n_2 \end{aligned} \quad (7)$$

(b) Use numerical solutions of the model (at judiciously chosen sets of parameter values) to explore how the stability of the interaction is affected as the value of q increases from 1. At parameters giving a stable equilibrium for $q = 1$, can increasing q destabilize the equilibrium and give rise to cycles? Conversely, at parameters giving rise to cycles when $q = 1$, can increasing q stabilize the equilibrium and eliminate the cycling?

7.2 The logs trick

In many biological models the state variables always must be non-negative, but a numerical ODE solver doesn't know this. If a variable decreases rapidly to near-zero values in the exact solution, a numerical

approximate solution might overshoot to a negative value, leading to nonsense. For example, if the number of infectives becomes negative in an SIR-type infectious disease model, the transmission rate βSI becomes negative (here β is a positive constant, S is the number of individuals susceptible to catching the disease, and I is the number of infective individuals). Disease transmission then goes in the wrong direction: contact between susceptibles and infectives makes infected individuals become healthy, pushing I even further negative. Once a model goes down the rabbit hole, it might never come back.

This problem can often be fixed by a simple trick that is often used but rarely written down. The trick is to transform the model onto natural log scale, solve the transformed model, and back-transform the output. This is easier than it sounds, because of the fact that for any state variable $x(t)$,

$$\frac{d(\log x(t))}{dt} = \frac{1}{x(t)} \frac{dx}{dt}. \quad (8)$$

This means that you can compute the untransformed vector field dx/dt , and then get the transformed vector field with a single element-by-element division. For example, here is the function that you would use to solve the Lotka-Volterra model on log scale:

```
Loglotka=function(t,logx,parms) {
  x=exp(logx);
  a=parms[1]; b=parms[2];
  xdot=rep(0,2);
  xdot[1]=x[1]*(2-x[1]-a*x[2]);
  xdot[2]=x[2]*(3-x[2]-b*x[1]);
  return(list(xdot/x));
}
```

There are only two differences from the original `lotka`: the first line that back-transforms from `logx` to `x`, and the last line that uses equation (8) to compute the vector field of the log-transformed state vector.

Or, with a bit more thinking, you can work out what $\frac{1}{x} \frac{dx}{dt}$ is, and write that as your function, as in:

```
Loglotka2=function(t,logx,parms) {
  a=parms[1]; b=parms[2]; x=exp(logx);
  xdot=rep(0,2);
  xdot[1]=(2-x[1]-a*x[2]);
  xdot[2]=(3-x[2]-b*x[1]);
  return(list(xdot));
}
```

The logs trick is not a panacea. It can even *create* problems that weren't there originally. If a positive state variable converges to 0 in non-transformed numerical solutions, then on log scale it is diverging to $-\infty$, potentially leading to numerical overflow errors. For more, see *Hurtado (2020)*.

Exercise 7.3 Write a script file that solves the Rosenzweig-MacArthur model (6) using the logs trick with `lsoda`, and use it to replicate your results from that exercise.

7.3 Additional arguments in `lsoda`

Sometimes, we need to fine-tune ODE solvers like `lsoda`. Some of the more common additional arguments to change are `rtol`, `atol`, `hmin`, and `hmax`.

rtol, **atol** control the accuracy that the solver tries to achieve (they stand for relative and absolute error tolerances). `lsoda` gets from one time-value to another by taking small steps, and adaptively adjusting their size (and number) to achieve the necessary accuracy, in particular so that the error in computing each new value of state variable x_i is less than $rtol|x_i| + atol$. Small values of `rtol` and `atol` give more accurate solutions, but it takes longer to get them.

hmin, **hmax** control the range of possible time-step sizes that can be used. Setting a value for `hmax` is just a bit of added security, to avoid `lsoda` becoming over-confident about how large a step it can take. This is most important when the model is explicitly time-dependent, and you want to make sure that `lsoda` doesn't jump over brief "shocks" to the system. Setting `hmin` is a way to ensure that `lsoda` doesn't grind down to taking infinitely many, infinitely short time steps.

8 Optimization and fitting models to data

Optimization is **extremely important** and **extremely difficult**. A typical problem for modelers is the following: given a set of data and a model, we want to choose model parameters to fit the data as well as possible. Here is an example: a data set $(x(t), t = 1, 2, \dots, 14)$ is stored in vectors **tvals**, **xvals** and we want to fit those data with a differential equation, the so-called θ -logistic model

$$dx/dt = rx(1 - (x/K)^\theta).$$

```
tvals=1:14;
xvals=c(15.58,30.04,66.05,141.6,274.6,410.0,468.8,526.4,472.5,
496.6,489.5,492.0,496.8,473.0);
```

```
ThetaLogist=function(t,x,parms) {
  r=parms[1]; K=100*parms[2]; theta=parms[3]
  xdot=r*x*(1-(x/K)^theta);
  return(list(xdot));
}
```

The first step is to choose an **objective function** $F(p)$ - a measure of how close the model is to the data, as a function of the parameter vector p . The objective function must be set up so that **small is beautiful** - a small value of F means a good fit to the data. One commonly used measure is the *least squares* criterion: choose parameters to minimize the sum of squared deviations between data and model output

```
TLfit=function(p) {
  parms=p[1:3]; x0=p[4]; times=1:14;
  out=lsoda(x0,times,ThetaLogist,parms,hmin=0.001);
  mse=mean((out[,2]-xvals)^2);
  return(mse);
}
```

Note that the model has 3 parameters, but the objective function **TLFit** has 4 arguments (i.e. p is a vector of length 4). The additional argument is the initial value x_0 . Were we to use `xvals[1]` as x_0 we would be giving that value special treatment, insisting that the model solution pass exactly through that value. To put all data points on an equal footing, we have to treat x_0 as another unknown value to estimate.

Now we want to minimize `TLFit` as a function of p . Calculus is no help: we can compute values of `TLfit` but there is no formula, so we can't use a "set derivatives to 0" approach. Instead we hand the problem

over to an **optimizer**, a routine that searches for the minimum of a function. Because optimization is important for lots of things – not just theoretical ecology, but really important things like devising delivery routes to provision each McDonalds “restaurant” at minimal expense – considerable effort has gone into developing software that can hunt efficiently for minima of functions. In R these are accessed through the functions **optim** and **nlm**. The former has the advantage of providing a common interface to several methods, so we will discuss **optim** here, but use of **nlm** is very similar. For the example above,

```
p0=c(1,5,1,15);
fit=optim(p0,TLfit);
fit2=optim(fit$par,TLfit);
fit$par; fit2$par;
```

p0 is our initial guess, based on eyeballing the data for r, K, x_0 and starting with a standard logistic ($\theta = 1$). The next line does a minimal call to **optim**, providing the objective function name and the initial guess, and accepting default values for everything else.

The default optimization method is the Nelder-Mead Simplex Algorithm, discussed below. This is a robust method intended for functions where it is costly to compute derivatives of the objective function, so it is best to search using only values of the objective function. As a safeguard, we re-optimize starting from the supposed minimum identified on the first call to **optim**, and check to see that we converge back to the same parameter estimates. In this case the re-optimization makes no significant adjustments to parameters, so we’re done and can plot the results (Figure 4) – see **FitThetaLogist.R** for the complete code.

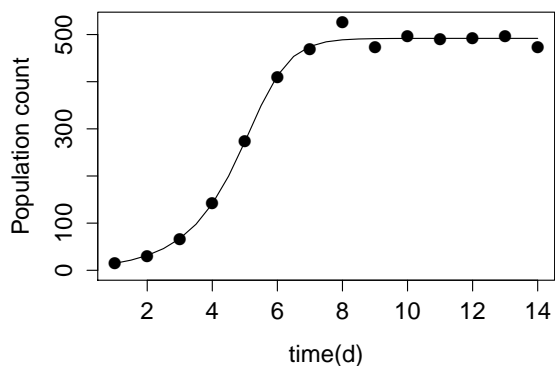


Figure 4: Results from least-squares fitting of the θ -logistic model. Points are the data (from Veilleux 1976,1979), curve is the model solution with best-fitting parameters

If simple optimization doesn’t seem to be working – as evidenced by the finding that repeated calls to **optim** keep on giving different results – it may help to vary some of the default parameters in **optim**.

Exercise 8.1 Type **names(fit)** at the console, and then use **?optim** to find out what all the parts are of the object returned by **optim**.

Exercise 8.2 If we reduce the number of parameters by assuming that $\theta = 1$ (a standard logistic model) can you fit the data as well? Modify the script file for the example so that $\theta = 1$, i.e. $dx/dt = rx(1-x/K)$,

and see if the model can fit the data as well as when we also allow θ to be fitted.

Exercise 8.3 Write a script file that uses `optim` to fit the same data as in the example above, by the difference equation model

$$x_{t+1} = \frac{\lambda x_t}{1 + b x_t}$$

[in plant ecology this is known as the Reciprocal Yield Law model]. Have your script produce a plot of data and fitted model like Figure (4). Note that instead of calling `lsoda` to solve the model, you will have to write a for-loop (inside the objective function) to compute solutions of the model. You'll also need an initial guess for the parameter values. The initial growth when x is small gives you an idea of what λ ought to be, and then you can estimate b so that the model's equilibrium corresponds to what you see in the data.

Note: The package `optimx` offers some improvements over the `optim` package, and additional optimization methods in R can be found in the CRAN Task View on Optimization at <https://cran.r-project.org/web/views/Optimization.html>.

8.1 What to optimize?

This is not an easy question, because it depends on what you believe about the real system. In the θ -logistic example above we asked for a single deterministic solution of the model to pass close to all the data points. This is called *calibration* or *trajectory matching*. It assumes that the real system is deterministic and that all differences between model output and the data are due to measurement errors. That is, we assume that the model is perfect but the data are not. In that case the objective function can be chosen to correspond to the statistical principle of **maximum likelihood**: parameters are chosen to maximize the likelihood of the observed data, based on the statistical distribution of the measurement errors.

The R function `mle`, in the `stats4` package, can be used to fit models by maximum likelihood. The script `FitThetaLogist.R` includes an example. The objective function for `mle` must be the negative log likelihood of the data under the assumed model. The fitted model then includes estimated standard errors for the parameter estimates, based on large-sample theory for maximum likelihood estimates. Unless you are sure that your data set is *really large*, the estimated standard errors should be viewed as rough approximations.

If the errors have a Normal distribution with constant variance, it is a standard result from statistics that maximum likelihood is equivalent to the least-squares objective function, as in the example above. Other assumptions about measurement errors lead to different objective functions. This is a topic in statistics so we will mention only one important case. If the errors have a Poisson distribution, which is often true or close-enough for population samples, then maximum likelihood is *approximately* equivalent to least-squares after transforming data and model to square-root scale. That is, for fitting with `optim` we would change the objective function `TLfit` in `FitThetaLogist.R` by redefining

```
mse=mean((sqrt(out[,2])-sqrt(xvals))^2)
```

For fitting with `mle` the `minuslogl` function is modified by setting

```
e2=sqrt(out[,2])-sqrt(xvals)
```

For more on fitting ODE models to data, see the book chapter *Hurtado (2020)*.

Exercise 8.4 Does this improved objective function make a difference in our θ -logistic example – that is, does the change in objective function result in any meaningful change in parameter estimates or the

fitted model solution? Modify the script file for the example, compute the parameter estimates with the modified objective function, and compare the two sets of parameter estimates.

Trajectory matching can run into problems if the true system is not deterministic. For example, consider a discrete-time model with random noise

$$X_{t+1} = F(X_t) + \sigma Z_t \quad (9)$$

where X_t is a vector of state variables, and Z_t is a vector of random perturbations to the state variable dynamics. The presence of random noise can change qualitative properties of model solutions. For example, a model that (in the absence of noise) would exhibit oscillatory convergence to a steady state, may instead exhibit fairly regular cycles. Fitting such data by trajectory matching will lead to incorrect parameters such that the model has stable periodic solutions in the absence of noise. Other fitting criteria are therefore more appropriate.

If error-free data are available on all state variables, then (9) is a nonlinear regression model, which can be fitted by any modern statistics package using nonlinear least squares (in R this is function `nls`). More typically one only has data on one or a few state variables. You can then try to choose parameters (including the noise level σ) so that model output matches overall features of the data such as the range of variation, periodicity of cycles if they occur, and the pattern of correlation between successive values. This is called “moment matching” or “method of moments” in the statistical literature. It suffers from the fact that the choice of which features to match is subjective, but has the advantage of that very few assumptions are needed about the underlying model, in order for parameter estimates to have good statistical properties.

Exercise 8.5 Here again is the Rosenzweig-MacArthur model

$$\begin{aligned} dn_1/dt &= r_1 n_1 (1 - n_1/K_1) - n_2 \frac{a_1 n_1}{B + n_1} \\ dn_2/dt &= n_2 \frac{a_2 n_1}{B + n_1} - r_2 n_2 \end{aligned} \quad (10)$$

Suppose that parameter values $r_1 = r_2 = 1$, $a_1 = 2$, $a_2 = 1.8$, $B = 200$ are known, and you have data showing the predators cycling regularly between a minimum value of about 95 and a maximum of about 205; you have no data on the prey. Write a script file to estimate K_1 by matching these features as closely as possible. That is, your objective function will take a single argument K_1 , generate solutions of the model, and return some measure of how well the model solutions match the observed features of the data. Since there is only one parameter to be fitted, for this exercise it will be sufficient to plot the objective function versus the value of K_1 , and see where it is minimized (for a more accurate result, see `?optimize`).

8.2 Controlling the optimization

Parameters affecting how `optim` proceeds can be set using the optional argument `control`, which is a list of options and their values. For example,

```
fit=optim(p0,TLfit,control=list(method="BFGS",maxit=1000,trace=4,parscale=p0));
```

Here we have:

- changed the optimization method to BFGS,
- set the maximum number of search steps to 1000,

- set the level of tracing to 4 (tracing means printing information to the console window as optimization proceeds, which is useful if things are going badly and you want to know why),
- told `optim` to scale parameters relative to the initial guess.

There are a lot of optional arguments – see `?optim`. Default values are well chosen except that the iteration limit `maxit` is suitable for “easy” problems where the function is not too wiggly or convoluted. If you often find that your safeguard optimization (`fit2` in the example above) is different from the first, try increasing the number of iterations. It is often helpful to use the `parscale` option. Internally `optim` works with parameters scaled relative to the corresponding value in `parscale`, which by default is a vector of 1’s. If you are using units are such that the elements of the optimal p are very different in magnitude – such as r and K in the last exercise – you can eliminate this problem by setting `parscale` to be your current best guess for the optimal p .

If optimization is generally working but takes a long time, you might try decreasing the error tolerances (`abstol` and `reltol` in `control`). `Optim` tries to find the minimum with the maximum possible accuracy (given the number of digits used to represent real numbers). Sometimes that results in a lot of time being spent making tiny, meaningless adjustments to parameter estimates (e.g. involving more significant digits than are reliable in the data).

Exercise 8.6 We need optimization for reasons besides parameter estimation. Consider a forager’s expected rate of energy gain $R(t_1, t_2)$ in a Patch Model with two patch types, travel time $T = 3$, 70% patches of type 1 with gain function $g_1(t) = 2t^{0.5}$, and 30% of type 2 with gain function $g_2(t) = t^{0.7}$. The code snippet below (from an old lab solution) defines the gain rate function:

```
g1=function(t1) {2*t1^0.5}
g2=function(t2) {t2^0.7}
gainR=function(t1,t2) {
  return((0.7*g1(t1)+0.3*g2(t2))/(3+0.7*t1+0.3*t2))
}
```

Write a script that uses `optim` to find the values (t_1^*, t_2^*) at which the rate of energy gain $R(t_1, t_2)$ is maximized, using the BFGS method. Recall that for `optim` the objective function must have one input argument, not two. Also recall that `optim` finds where a function is minimized; to find where a function $F(x)$ is maximized you can use $-F(x)$ as the objective function.

8.3 How to optimize

This discussion is based on Kelley (1999), the optimization chapter in Numerical Recipes (available at www.library.cornell.edu/nr and www.nr.com), and much painful experience fitting models to data.

The basic decision in optimization is how you want to get from your initial guess to a final value: a few clever steps in parameter space, or a lot of simple steps. Being “clever” means using a lot of information about the function, either computed at each new evaluation point (e.g. its derivatives and possibly second derivatives with respect to each argument) or else built up gradually over the search for the minimum. Using this information the algorithm tries to identify a good direction in which to search for a local minimum. For example, the first and second derivatives at the current evaluation point define a quadratic approximation to the objective function. But rather than jumping directly to the minimum of the quadratic approximation, the algorithm does a one-dimensional search along the line connecting the current evaluation point and the minimum of the quadratic approximation. The point on that line where the function value is smallest (as approximated by a one-dimensional minimization algorithm) is then used as the next evaluation point. Methods of this type in `optim` include **BFGS** and **L-BFGS-B**. Both of these use derivatives of the objective function, either supplied by the user as a function or else computed numerically by forming difference quotients, and build up an approximate second derivative as the function and its derivative are repeatedly evaluated.

Cleverness is often counterproductive, however, because your function may have *multiple local optima* that are “worse” than the desired (global) optimum. To find the global minimum you then have to repeat the optimization many times, starting from different initial points. The efficiency of each repetition is often more than outweighed by the need to run many repetitions.

Less clever method often fare better against multiple local minima. They work by gradually narrowing in on a minimum, so initially they don’t pay much attention to the objective function’s fine-scale structure (Kelley 1999). The most popular method of this type is the Nelder-Mead Simplex Algorithm. Initially, values of the function are computed at a set of points (a *simplex*) surrounding the initial guess, n points for a function of n variables. At each step, the algorithm tries to replace the worst point (the one with the highest function value) with a better one, by searching along the line between the worst point and the average of all the others. If that fails, it may shrink the simplex down around the best point on the current simplex.

You can also use the “multi-start” method of picking your favorite algorithm (e.g., Nelder-Mead) and running it in parallel starting from multiple initial values.

However there really is no cure for the problem of multiple local minima. To be confident of your results you need to run the optimization from multiple starting points and make sure that you repeatedly find the same “best” minimum, and always re-start the optimization from the supposed minimum to make sure that you converge back to it.

For more on Optimization in R please see the CRAN Task View on Optimization and Mathematical Programming at <https://cran.r-project.org/web/views/Optimization.html>.

9 Document Creation in Rstudio

Turning in nicely formatted and typed homework solutions or reports for an employer often involves running R scripts, saving output like figures and tables, then importing them into a document like an MS Word or \LaTeX document.

There are, however, at least two ways of embedding your R analyses into those documents so that you can skip the steps of importing R output into your final document, as well as include nicely formatted R code in that document.

9.1 R Markdown

The first (and probably the easiest, unless you already know some \LaTeX) is to create an R Markdown document. In Rstudio, just go to **File > New File > R Markdown...** to generate a new template, and visit the URL included in that template to get started. I also recommend the old version of the R Markdown cheat sheet (the new one is also worth looking at) available at <https://www.rstudio.com/resources/cheatsheets/>.

9.2 knitr/Sweave Documents (\LaTeX with embedded R code & output)

The second option is best suited to those who already are comfortable using \LaTeX . These **knitr** documents (a re-imagined improvement of **Sweave**) are essentially \LaTeX documents with inserted ‘code blocks’ almost identical to the code blocks discussed in the R Markdown documentation. This allows a document author to create a \LaTeX document and insert snippets of R code, which is then automatically parsed and the code and output nicely formatted without any further intervention by the author (e.g., the book chapter *Hurtado (2020)* was created this way). To get started, you’ll want to follow the \LaTeX and R/Rstudio

installation instructions at <https://www.pauljhurtado.com/teaching/software.html>. I have provided some knitr template documents, a link to which can be found at <https://www.pauljhurtado.com/latex/>.

Note that `knitr` documents can also run and format the output of code written in other languages (e.g., Python) and not only R! This can be done so long as the `knitr` package in R is able to call that other software to run the embedded code. For details see <https://bookdown.org/yihui/rmarkdown-cookbook/eng-python.html> in the *R Markdown Cookbook* by Yihui Xie, Christophe Dervieux, and Emily Riederer.

References

- G. Fussmann, S.P. Ellner, K.W. Shertzer, and N.G. Hairston, Jr. 2000. Crossing the Hopf bifurcation in a live predator-prey system. *Science* 290: 1358 - 1360. DOI:[10.1126/science.290.5495.1358](https://doi.org/10.1126/science.290.5495.1358)
- Hurtado, P.J. 2020. Building New Models: Rethinking and Revising ODE Model Assumptions. In: Callender Highlander H., Capaldi A., Diaz Eaton C. (eds) *An Introduction to Undergraduate Research in Computational and Mathematical Biology*. Foundations for Undergraduate Research in Mathematics. Birkhäuser, Cham. DOI:[10.1007/978-3-030-33645-5_1](https://doi.org/10.1007/978-3-030-33645-5_1)
- Ihaka, R., and R. Gentleman. 1996. R: A language for data analysis and graphics. *Journal of Computational and Graphical Statistics* 5(3) pp. 299-314. DOI:[10.2307/1390807](https://doi.org/10.2307/1390807)
- Kelley, C.T. *Iterative Methods for Optimization*. SIAM (Society for Industrial and Applied Mathematics), Philadelphia PA.
- Maindonald, J.H. 2004. *Using R for Data Analysis and Graphics: Introduction, Code, and Commentary*. URL <http://www.cran.R-project.org>.
- Press, W.H., S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery. *Numerical Recipes: the Art of Scientific Computing*, 2nd edition. Cambridge University Press (complete editions for C, f77, and f90 are available online at www.nr.com).
- R Core Team (2017). *R: A language and environment for statistical computing*. R Foundation for Statistical Computing, Vienna, Austria. URL <https://www.R-project.org/>.
- Verzani, J. 2002. *simpleR – using R for Introductory Statistics*. URL <http://www.cran.R-project.org>.
- Veilleux, B. G. 1976. The analysis of a predatory interaction between *Didinium* and *Paramecium*. Master's thesis, University of Alberta.
- Veilleux, B. G. 1979. An analysis of the predatory interaction between *Paramecium* and *Didinium* *Journal of Animal Ecology* 4: 787-803.